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Dedicated to

Mary,

whose memory I will cherish forever.

V. KOPSKÝ

Tikva (זכרונה לברכה) and Professor W. Opechowski,

may their memories be blessed.

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Preface

By V. Kopský and D. B. Litvin

This volume is divided into two sections. The first, covered in Parts 1–4, can be considered as an extension of Volume A: *Space-Group Symmetry*, in this series of *International Tables for Crystallography*. As Volume A treats one-, two-, and three-dimensional space groups, this Volume treats the two- and three-dimensional subperiodic groups. That is, it treats the frieze groups, two-dimensional groups with one-dimensional translations, the rod groups, three-dimensional groups with one-dimensional translations, and layer groups, three-dimensional groups with two-dimensional translations. A reader familiar with Volume A should readily recognize the format and content of the tables of Parts 1–4 of this volume. The information presented for the subperiodic groups is in the same format and consists of the same content as that provided in Volume A for space groups.

A relationship between space and subperiodic groups is considered in Parts 5 and 6: given a crystal of a specific space-group symmetry and a plane transecting the crystal, one can enquire as to what is the layer subgroup of the space group which leaves this plane invariant. The physical motivation for answering this question is discussed in Chapter 5.2. This is followed by the 'Scanning Tables' in which the layer symmetries of 'sectional' planes are tabulated for all crystallographic orientations and for all positions (locations) of these planes. These tables also contain explicitly the orbits of these planes and implicitly, *via* the so-called 'scanning groups', information about the rod symmetries of straight lines which penetrate through the crystal.

A new feature of this second edition is the addition of Seitz notation. In the symmetry-operations section of each table in Parts 2–4 the Seitz notation for each symmetry operation is given below its geometric notation. Minor additions to the text and tables, and corrections of a few typographical errors, have been made.

The history of this work dates back to 1972 when one of us (DBL) was asked by a fellow post doc, John Berlinsky, if there existed International-like tables to classify arrays of hydrogen molecules on a surface with the molecules not constrained to be 'in-plane'. Tables for the layer groups were subsequently derived in the content and format of the *International Tables for X-ray Crystallography*, Volume 1 (1952). It was later pointed out by a referee of *Acta Crystallographica* that such tables had already been published by E. Wood in 1964. Work on these tables remained dormant until 1983 with the publication of Volume A of *International Tables for Crystallography*, and the extensive addition of new features in the description of each space group. Work began then on including these new features into tables for the layer groups.

During this same time one of us (VK) was asked by Dr V. Janovec to investigate the group-theoretical aspects of the analysis of domain walls and twin boundaries. Thus, work began on the relationships between space groups and subperiodic groups and standards for the subperiodic groups.

It is our subsequent collaboration which has led to the material presented in this volume. In the many decisions concerning the choice of symbols, origins and settings for the subperiodic groups, the final choices were made based on relationships between space groups and subperiodic groups. While these relationships are not all explicitly given here, they have been implicitly used.

As with any major work such as this, there are those to whom we must give our thanks: Dr E. Woods is thanked for her encouragement during the initial stage of this work. Dr Th. Hahn has provided advice, comments and encouragement dating back to 1983. Constructive feedback on reading parts of this work were received from Drs Th. Hahn, H. Wondratschek and V. Janovec. The drawings in Parts 1–4 of this volume were done by Steven Erb, a Mechanical Engineering Technology student at the Berks Campus of the Pennsylvania State University. The drawings in Parts 5 and 6 were done by V. Kopský Jr, a biology student at Charles University. We also thank M. I. Aroyo, P. Konstantinov, E. Kroumova and M. Gateshki for converting the computer files of Parts 2, 3 and 4 from WordPerfect to LaTeX format.

The financial support received from various organizations during which work was performed leading to and for this volume from a National Academy of Science–Czechoslovak Academy of Science Exchange Program (1984), the United States National Science Foundation (INT-8922251), the International Union of Crystallography and the Pennsylvania State University is gratefully acknowledged by us. In addition, for their major additional support DBL thanks the United States National Science Foundation (DMR-8406196, DMR-9100418, DMR-9305825 and DMR-9510335) and VK the University of the South Pacific (Fiji) (Research Committee Grant 070-91111), under which a major portion of this work was completed in an idyllic setting, and the Grant Agency of the Czech Republic (GA CR 202/96/1614).

As to the dedication, we would like to point out, to quell any rumours to the contrary, that Mary and Tikva (זכרונה לברכה) are our respective wives. Their unending patience and constant encouragement are indeed due recognition. The parenthetical Hebrew means 'may her memory be blessed', and Professor W. Opechowski is included as DBL's scientific 'father'.

1.1. Symbols and terms used in Parts 1–4

In this chapter the crystallographic symbols and terms that occur in the tables and the text of Parts 1–4 of this volume are defined. The symbols and definitions given below in Tables 1.1.1 to 1.1.3 follow those given in Part 1 of Volume A of *International Tables for Crystallography* (2005).

Table 1.1.1. *Printed symbols for crystallographic items*

Printed symbol	Explanation
a; **b**; **c**	Basis vectors of direct lattice
a; *b*; *c*	Length of basis vectors
α; β; γ	Interaxial (lattice) angles **b**∧**c**, **c**∧**a**, **a**∧**b**
a′; **b**′; **c**′	New basis vectors after a transformation of the basis vectors
(*abc*)	Setting symbol, notation for the transformation of the basis vectors, *e.g.* ($b\bar{a}c$) means **a**′ = **b**, **b**′ = −**a** and **c**′ = **c**
r	Position vector of a point or an atom
x, *y*, *z*	Coordinates of a point or location of an atom expressed in units of *a*, *b* and *c*; coordinates of the end point of the position vector **r**
*x***a**; *y***b**; *z***c**	Components of the position vector **r**
[*uvw*]	Indices of a three-dimensional lattice direction
[*uv*]	Indices of a two-dimensional lattice direction
(*hkl*)	Miller indices

Table 1.1.2. *Printed symbols for symmetry elements and for the corresponding symmetry operations*

Printed symbol	Symmetry element and its orientation	Generating symmetry operation with glide or screw vector
m	Reflection plane, mirror plane (three dimensions)	Reflection through a plane
	Reflection line, mirror line (two dimensions)	Reflection through a line
a, *b* or *c*	'Axial' glide plane	Glide reflection through a plane, with glide vector
a	⊥[010] or ⊥[001]	$\frac{1}{2}$**a**
b	⊥[100] or ⊥[001]	$\frac{1}{2}$**b**
c	⊥[100] or ⊥[010]	$\frac{1}{2}$**c**
	⊥[1$\bar{1}$0] or ⊥[110]	$\frac{1}{2}$**c**
	⊥[100] or ⊥[010] or ⊥[$\bar{1}\bar{1}$0]	$\frac{1}{2}$**c**, hexagonal coordinate system
	⊥[1$\bar{1}$0] or ⊥[120] or ⊥[$\bar{2}\bar{1}$0]	$\frac{1}{2}$**c**, hexagonal coordinate system
n	'Diagonal' glide plane (in noncentred cells only) ⊥[001]	Glide reflection through a plane, with glide vector $\frac{1}{2}$(**a** + **b**)
e	'Double' glide plane ⊥[001] (in centred cells only)	Two glide reflections through planes with glide vectors $\frac{1}{2}$**a** and $\frac{1}{2}$**b**
g	Glide line (two dimensions)	Glide reflection through a line, with glide vector
	⊥[01]; ⊥[10]	$\frac{1}{2}$**a**; $\frac{1}{2}$**b**
1	None	Identity
2, 3, 4, 6	*n*-fold rotation axis, *n* (three dimensions)	Counterclockwise rotation of 360/*n* degrees about an axis
	n-fold rotation point, *n* (two dimensions)	Counterclockwise rotation of 360/*n* degrees about a point
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through a point
$\bar{2} = m$, $\bar{3}$, $\bar{4}$, $\bar{6}$	Rotoinversion axis, $\bar{n}$	Counterclockwise rotation of 360/*n* degrees around an axis, followed by inversion through a point on the axis
2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5	*n*-fold screw axes, n_p	Right-handed screw rotation of 360/*n* degrees around an axis, with screw vector (p/n)*t*; *t* is the shortest translation vector parallel to the axis in the direction of the screw

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Table 1.1.3. *Graphical symbols*

(*a*) Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions).

Symmetry plane or symmetry line	Graphical symbol	Glide vectors in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
Mirror plane, mirror line		None	*m*
Glide plane, glide line		$\frac{1}{2}$ along line parallel to projection plane; $\frac{1}{2}$ along line in plane	*a*, *b* or *c*; *g*
Glide plane		$\frac{1}{2}$ normal to projection plane	*c*

(*b*) Symmetry planes parallel to plane of projection.

Symmetry plane	Graphical symbol	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Mirror plane		None	*m*
Glide plane		$\frac{1}{2}$ in the direction of arrow	*a*, *b* or *c*
'Double' glide plane		Two glide vectors; $\frac{1}{2}$ in either of the directions of the two arrows	*e*
'Diagonal' glide plane		$\frac{1}{2}$ in the direction of the arrow	*n*

(*c*) Symmetry axes normal to the plane of projection (three dimensions) and symmetry points in the plane of the figure (two dimensions).

Symmetry axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Twofold rotation axis, twofold rotation point		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Fourfold rotation axis		None	4
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3
Sixfold rotation axis		None	6

Table 1.1.3 (*cont.*)

Symmetry axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Sixfold screw axis: '6 sub 1'		$\frac{1}{6}$	6_1
Sixfold screw axis: '6 sub 2'		$\frac{1}{3}$	6_2
Sixfold screw axis: '6 sub 3'		$\frac{1}{2}$	6_3
Sixfold screw axis: '6 sub 4'		$\frac{2}{3}$	6_4
Sixfold screw axis: '6 sub 5'		$\frac{5}{6}$	6_5
Centre of symmetry, inversion centre: '1 bar'		None	$\bar{1}$
Twofold rotation axis with centre of symmetry		None	$2/m$
Twofold screw axis with centre of symmetry		$\frac{1}{2}$	$2_1/m$
Inversion axis: '3 bar'		None	$\bar{3}$
Inversion axis: '4 bar'		None	$\bar{4}$
Fourfold rotation axis with centre of symmetry		None	$4/m$
'4 sub 2' screw axis with centre of symmetry		$\frac{1}{2}$	$4_2/m$
Inversion axis: '6 bar'		None	$\bar{6}$
Sixfold rotation axis with centre of symmetry		None	$6/m$
'6 sub 3' screw axis with centre of symmetry		$\frac{1}{2}$	$6_3/m$

(*d*) Symmetry axes parallel to plane of projection.

Symmetry axis	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Twofold rotation axis		None	2
Twofold screw axis		$\frac{1}{2}$	2_1

References

International Tables for Crystallography (2005). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Heidelberg: Springer. [Previous editions: 1983, 1987, 1992, 1995 and 2002. Abbreviated as *IT* A (2005).]

1.2. Guide to the use of the subperiodic group tables

This present volume is, in part, an extension of *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 2005). Symmetry tables are given in *IT* A for the 230 three-dimensional crystallographic space-group types (space groups) and the 17 two-dimensional crystallographic space-group types (plane groups). We give in the following three parts of this volume analogous symmetry tables for the two-dimensional and three-dimensional subperiodic group types: the seven crystallographic *frieze-group* types (two-dimensional groups with one-dimensional translations) in Part 2; the 75 crystallographic *rod-group* types (three-dimensional groups with one-dimensional translations) in Part 3; and the 80 crystallographic *layer-group* types (three-dimensional groups with two-dimensional translations) in Part 4. This chapter forms a guide to the entries of the subperiodic group tables given in Parts 2–4.

1.2.1. Classification of subperiodic groups

Subperiodic groups can be classified in ways analogous to the space groups. For the mathematical definitions of these classifications and their use for space groups, see Chapter 8.2 of *IT* A (2005). Here we shall limit ourselves to those classifications which are explicitly used in the symmetry tables of the subperiodic groups.

1.2.1.1. Subperiodic group types

The subperiodic groups are classified into *affine subperiodic group types*, *i.e.* affine equivalence classes of subperiodic groups. There are 80 affine layer-group types and seven affine frieze-group types. There are 67 crystallographic and an infinity of noncrystallographic (Opechowski, 1986) affine rod-group types. We shall consider here only rod groups of the 67 crystallographic rod-group types. We shall refer here to these crystallographic affine rod-group types simply as affine rod-group types and to the crystallographic rod groups belonging to these types simply as rod groups.

The subperiodic groups are also classified into *proper affine subperiodic group types*, *i.e.* proper affine classes of subperiodic groups. For layer and frieze groups, the two classifications are identical. For rod groups, each of eight affine rod-group types splits into a pair of *enantiomorphic crystallographic rod-group types*. Consequently, there are 75 proper affine rod-group types. The eight pairs of enantiomorphic rod-group types are $\not{p}4_1$ (R24), $\not{p}4_3$ (R26); $\not{p}4_122$ (R31), $\not{p}4_322$ (R33); $\not{p}3_1$ (R43), $\not{p}3_2$ (R44); $\not{p}3_112$ (R47), $\not{p}3_212$ (R48); $\not{p}6_1$ (R54), $\not{p}6_5$ (R58); $\not{p}6_2$ (R55), $\not{p}6_4$ (R57); $\not{p}6_122$ (R63), $\not{p}6_522$ (R67); and $\not{p}6_222$ (R64), $\not{p}6_422$ (R66). (Each subperiodic group is given in the text by its Hermann–Mauguin symbol followed in parenthesis by a letter L, R or F to denote it, respectively, as a layer, rod or frieze group, and its sequential numbering from Parts 2, 3 or 4.) We shall refer to the proper affine subperiodic group types simply as subperiodic group types.

1.2.1.2. Other classifications

There are 27 geometric crystal classes of layer groups and rod groups, and four geometric crystal classes of frieze groups. These are listed, for layer groups, in the fourth column of Table 1.2.1.1, and for the rod and frieze groups in the second columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

We further classify subperiodic groups according to the following classifications of the subperiodic group's point group and lattice group. These classifications are introduced to emphasize the relationships between subperiodic groups and space groups:

(1) The point group of a layer or rod group is three-dimensional and corresponds to a point group of a three-dimensional space group. The point groups of three-dimensional space groups are classified into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic crystal systems. We shall use this classification also for subperiodic groups. Consequently, the three-dimensional subperiodic groups are classified, see the third column of Table 1.2.1.1 and the first column of Table 1.2.1.2, into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal crystal systems. The cubic crystal system does not arise for three-dimensional subperiodic groups. Two-dimensional subperiodic groups, *i.e.* frieze groups, are analogously classified, see the first column of Table 1.2.1.3, into the oblique and rectangular crystal systems.

(2) The two-dimensional lattice of a layer group is also a two-dimensional lattice of a plane group. The lattices of plane groups are classified, according to *Bravais* (*flock*) *systems*, see *IT* A (2005), into the oblique, rectangular, square and hexagonal Bravais systems. We shall also use this classification for layer groups, see the first column in Table 1.2.1.1. For rod and frieze groups no lattice classification is used, as all one-dimensional lattices form a single Bravais system.

A subdivision of the monoclinic rod-group category is made into monoclinic/inclined and monoclinic/orthogonal. Two different coordinate systems, see Table 1.2.1.2, are used for the rod groups of these two subdivisions of the monoclinic crystal system. These two coordinate systems differ in the orientation of the plane containing the non-lattice basis vectors relative to the lattice vectors. For the monoclinic/inclined subdivision, the plane containing the non-lattice basis vectors is, see Fig. 1.2.1.1, *inclined* with respect to the lattice basis vector. For the monoclinic/orthogonal subdivision, the plane is, see Fig. 1.2.1.2, *orthogonal*.

1.2.1.2.1. Conventional coordinate systems

The subperiodic groups are described by means of a *crystallographic coordinate system* consisting of a *crystallographic origin*, denoted by *O*, and a *crystallographic basis*. The basis vectors for the three-dimensional layer groups and rod groups are labelled **a**, **b** and **c**. The basis vectors for the two-dimensional frieze groups are labelled **a** and **b**. Unlike space groups, not all basis vectors of the crystallographic basis are lattice vectors. Like space groups, the crystallographic coordinate system is used to define the symmetry operations (see Section 1.2.9) and the Wyckoff positions (see Section 1.2.11). The symmetry operations are defined with respect to the directions of both lattice and non-lattice basis vectors. A Wyckoff position, denoted by a coordinate triplet (x, y, z) for the three-dimensional layer and rod groups, is

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Table 1.2.1.1. *Classification of layer groups*

Bold or bold underlined symbols indicate Laue groups. Bold underlined point groups are also lattice point symmetries (holohedries).

Two-dimensional Bravais system	Symbol	Three-dimensional crystal system	Crystallographic point groups	No. of layer-group types	Restrictions on conventional coordinate system	Cell parameters to be determined	Bravais lattice
Oblique	*m*	Triclinic	1, $\bar{\mathbf{1}}$	2	None	*a*, *b*, γ†	*mp*
		Monoclinic	2, *m*, **2/*m***	5	$\alpha = \beta = 90°$		
Rectangular	*o*			11	$\beta = \gamma = 90°$	*a*, *b*	*op*
		Orthorhombic	222, 2*mm*, ***mmm***	30	$\alpha = \beta = \gamma = 90°$		*oc*
Square	*t*	Tetragonal	4, $\bar{4}$, **4/*m*** 422, 4*mm*, $\bar{4}$2*m*, ***4/mmm***	16	$a = b$ $\alpha = \beta = \gamma = 90°$	*a*	*tp*
Hexagonal	*h*	Trigonal	3, $\bar{\mathbf{3}}$ 32, 3*m*, $\bar{\mathbf{3}}$***m***	8	$a = b$	*a*	*hp*
		Hexagonal	6, $\bar{6}$, **6/*m*** 622, 6*mm*, $\bar{6}$*m*2, ***6/mmm***	8	$\gamma = 120°$ $\alpha = \beta = 90°$		

† This angle is conventionally taken to be non-acute, *i.e.* $\geq 90°$.

Table 1.2.1.2. *Classification of rod groups*

Bold symbols indicate Laue groups.

Three-dimensional crystal system	Crystallographic point groups	No. of rod-group types	Restrictions on conventional coordinate system
Triclinic	1, $\bar{\mathbf{1}}$	2	None
Monoclinic (inclined)	2, *m*, **2/*m***	5	$\beta = \gamma = 90°$
Monoclinic (orthogonal)		5	$\alpha = \beta = 90°$
Orthorhombic	222, 2*mm*, ***mmm***	10	$\alpha = \beta = \gamma = 90°$
Tetragonal	4, $\bar{4}$, **4/*m*** 422, 4*mm*, $\bar{4}$2*m*, ***4/mmm***	19	
Trigonal	3, $\bar{\mathbf{3}}$ 32, 3*m*, $\bar{\mathbf{3}}$***m***	11	$\alpha = \beta = 90$, $\gamma = 120°$
Hexagonal	6, $\bar{6}$, **6/*m*** 622, 6*mm*, $\bar{6}$*m*2, ***6/mmm***	23	

Table 1.2.1.3. *Classification of frieze groups*

Bold symbols indicate Laue groups.

Two-dimensional crystal system	Crystallographic point groups	No. of frieze-group types	Restrictions on conventional coordinate system
Oblique	1, **2**	2	None
Rectangular	*m*, ***2mm***	5	$\gamma = 90°$

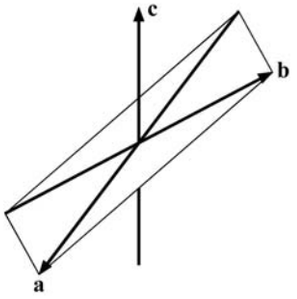

Fig. 1.2.1.1. Monoclinic/inclined basis vectors. For the monoclinic/inclined subdivision, $\beta = \gamma = 90°$ and the plane containing the **a** and **b** non-lattice basis vectors is *inclined* with respect to the lattice basis vector **c**.

defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$. For the two-dimensional frieze groups, a Wyckoff position is denoted by a coordinate doublet (x, y) and is defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b}$.

The term *setting* will refer to the assignment of the labels **a**, **b** and **c** (and the corresponding directions [100], [010] and [001], respectively) to the basis vectors of the crystallographic basis (see Section 1.2.6). In the *standard setting*, those basis vectors which are also lattice vectors are labelled as follows: for layer groups with their two-dimensional lattice by **a** and **b**, for rod groups with their one-dimensional lattice by **c**, and for frieze groups with their one-dimensional lattice by **a**.

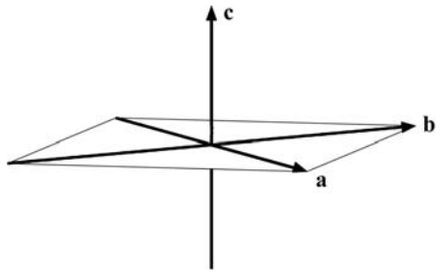

Fig. 1.2.1.2. Monoclinic/orthogonal basis vectors. For the monoclinic/orthogonal subdivision, $\alpha = \beta = 90°$ and the plane containing the **a** and **b** non-lattice basis vectors is *orthogonal* to the lattice basis vector **c**.

The selection of a crystallographic coordinate system is not unique. Following *IT* A (2005), we choose *conventional crystallographic coordinate systems* which have a right-handed set of basis vectors and such that symmetry of the subperiodic groups is best displayed. The conventional crystallographic coordinate systems used in the standard settings are given in the sixth column of Table 1.2.1.1 for the layer groups, and the fourth columns of Tables 1.2.1.2 and 1.2.1.3 for the rod groups and frieze groups, respectively. The crystallographic origin is conventionally chosen at a centre of symmetry or at a point of high site symmetry (see Section 1.2.7).

The *conventional unit cell* of a subperiodic group is defined by the crystallographic origin and by those basis vectors which are also lattice vectors. For layer groups in the standard setting, the cell parameters, the magnitude of the lattice basis vectors **a** and **b**, and the angle between them, which specify the conventional cell, are given in the seventh column of Table 1.2.1.1. The conventional unit cell obtained in this manner turns out to be either *primitive* or *centred* and is denoted by *p* or *c*, respectively, in the eighth column of Table 1.2.1.1. For rod and frieze groups with their one-dimensional lattices, the single cell parameter to be specified is the magnitude of the lattice basis vector.

1.2.2. Contents and arrangement of the tables

The presentation of the subperiodic group tables in Parts 2, 3 and 4 follows the form and content of *IT* A (2005). The entries for a subperiodic group are printed on two facing pages or continuously on a single page, where space permits, in the following order (deviations from this standard format are indicated on the relevant pages):

Left-hand page:

(1) *Headline*;

(2) *Diagrams* for the symmetry elements and the general position;

(3) *Origin*;

(4) *Asymmetric unit*;

(5) *Symmetry operations*.

Right-hand page:

(6) *Headline* in abbreviated form;

(7) *Generators selected*: this information is the basis for the order of the entries under *Symmetry operations* and *Positions*;

(8) General and special *Positions*, with the following columns: *Multiplicity*; *Wyckoff letter*; *Site symmetry*, given by the oriented site-symmetry symbol; *Coordinates*; *Reflection conditions*;

(9) *Symmetry of special projections*;

(10) *Maximal non-isotypic non-enantiomorphic subgroups*;

(11) *Maximal isotypic subgroups and enantiomorphic subgroups of lowest index*;

(12) *Minimal non-isotypic non-enantiomorphic supergroups*.

1.2.2.1. Subperiodic groups with more than one description

For two monoclinic/oblique layer-group types with a glide plane, more than one description is available: *p*11*a* (L5) and *p*112/*a* (L7). The synoptic descriptions consist of abbreviated treatments for three 'cell choices', called 'cell choices 1, 2 and 3' [see Section 1.2.6, (i) *Layer groups*]. A complete description is given for cell choice 1 and it is repeated among the synoptic descriptions of cell choices 2 and 3. For three layer groups, *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), two descriptions are given (see Section 1.2.7). These two descriptions correspond to the choice of origin, at an inversion centre and on a fourfold axis. For 15 rod-group types, two descriptions are given, corresponding to two settings [see Section 1.2.6, (ii) *Rod groups*].

1.2.3. Headline

The description of a subperiodic group starts with a headline on a left-hand page, consisting of two or three lines which contain the following information when read from left to right.

First line:

(1) The *short international* (Hermann–Mauguin) *symbol* of the subperiodic group type. Each symbol has two meanings. The first is that of the Hermann–Mauguin symbol of the subperiodic group type. The second meaning is that of a specific subperiodic group which belongs to this subperiodic group type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 1.2.9) given on the page headed by that Hermann–Mauguin symbol, or by the given list of general positions (see Section 1.2.11). Alternatively, this group is defined by the given diagrams (see Section 1.2.6). The Hermann–Mauguin symbols for the subperiodic group types are distinct except for the rod- and frieze-group types $\not{p}1$ (R1, F1), $\not{p}211$ (R3, F2) and $\not{p}11m$ (R10, F4).

(2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric class to which the subperiodic group belongs.

(3) The name used in classifying the subperiodic group types. For layer groups this is the combination crystal system/Bravais system classification given in the first two columns of Table 1.2.1.1, and for rod and frieze groups this is the crystal system classification in the first columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

Second line:

(4) The sequential number of the subperiodic group type.

(5) The *full international* (Hermann–Mauguin) *symbol* for the subperiodic group type.

(6) The *Patterson symmetry*.

Third line:

This line is used to indicate the cell choice in the case of layer groups *p*11*a* (L5) and *p*112/*a* (L7), the origin choice for the three layer groups *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), and the setting for the 15 rod groups with two distinct Hermann–Mauguin setting symbols (see Table 1.2.6.2).

1.2.4. International (Hermann–Mauguin) symbols for subperiodic groups

Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the subperiodic group.

(i) The letters for the two centring types for layer groups are the lower-case italic letter *p* for a primitive cell and the lower-case

Table 1.2.4.1. *Sets of symmetry directions and their positions in the Hermann–Mauguin symbol*

In the standard setting, periodic directions are [100] and [010] for the layer groups, [001] for the rod groups, and [10] for the frieze groups.

(*a*) Layer groups and rod groups.

	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100] [010]	[1$\bar{1}$0] [110]
Trigonal Hexagonal	[001]	[100] [010] [$\bar{1}\bar{1}$0]	[1$\bar{1}$0] [120] [$\bar{2}\bar{1}$0]

(*b*) Frieze groups.

	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Oblique	Rotation point in plane		
Rectangular		[10]	[01]

italic letter *c* for a centred cell. For rod and frieze groups there is only one centring type, the one-dimensional primitive cell, which is denoted by the lower-case script letter $\not p$.

(ii) The one or three entries after the centring letter refer to the one or three kinds of *symmetry directions* of the conventional crystallographic basis. Symmetry directions occur either as singular directions or as sets of symmetrically equivalent symmetry directions. Only one representative of each set is given. The sets of symmetry directions and their sequence in the Hermann–Mauguin symbol are summarized in Table 1.2.4.1.

Each position in the Hermann–Mauguin symbol contains one or two characters designating symmetry elements, axes and planes that occur for the corresponding crystallographic symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters are separated by a slash, *e.g.* the 4/*m* in $\not p$4/*mcc* (R40). Crystallographic symmetry directions that carry no symmetry elements are denoted by the symbol '1', *e.g.* *p*3*m*1 (L69) and *p*112 (L2). If no misinterpretation is possible, entries '1' at the end of the symbol are omitted, as in *p*4 (L49) instead of *p*411. Subperiodic groups that have in addition to translations no symmetry directions or only centres of symmetry have only one entry after the centring letter. These are the layer-group types *p*1 (L1) and *p*$\bar{1}$ (L2), the rod-group types $\not p$1 (R1) and $\not p\bar{1}$ (R2), and the frieze group $\not p$1 (F1).

1.2.5. Patterson symmetry

The entry *Patterson symmetry* in the headline gives the subperiodic group of the *Patterson function*, where Friedel's law is assumed, *i.e.* with neglect of anomalous dispersion. [For a discussion of the effect of dispersion, see Fischer & Knof (1987) and Wilson (2004).] The symbol for the Patterson subperiodic group can be deduced from the symbol of the subperiodic group in two steps:

(i) Glide planes and screw axes are replaced by the corresponding mirror planes and rotation axes.

Table 1.2.5.1. *Patterson symmetries for subperiodic groups*

(*a*) Layer groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
$\bar{1}$	*p*	*p*$\bar{1}$ (L2)
112/*m*	*p*	*p*112/*m* (L6)
2/*m*11	*p*, *c*	*p*2/*m*11 (L14), *c*2/*m*11 (L18)
mmm	*p*, *c*	*pmmm* (L37), *cmmm* (L47)
4/*m*	*p*	*p*4/*m* (L51)
4/*mmm*	*p*	*p*4/*mmm* (L61)
$\bar{3}$	*p*	*p*$\bar{3}$ (L66)
$\bar{3}$1*m*	*p*	*p*$\bar{3}$1*m* (L71)
$\bar{3}$*m*1	*p*	*p*$\bar{3}$*m*1 (L72)
6/*m*	*p*	*p*6/*m* (L75)
6/*mmm*	*p*	*p*6/*mmm* (L80)

(*b*) Rod groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
$\bar{1}$	$\not p$	$\not p\bar{1}$ (R2)
2/*m*11	$\not p$	$\not p$2/*m*11 (R6)
112/*m*	$\not p$	$\not p$112/*m* (R11)
mmm	$\not p$	$\not p$*mmm* (R20)
4/*m*	$\not p$	$\not p$4/*m* (R28)
4/*mmm*	$\not p$	$\not p$4/*mmm* (R39)
$\bar{3}$	$\not p$	$\not p\bar{3}$ (R48)
$\bar{3}$*m*	$\not p$	$\not p\bar{3}$1*m* (R51)
6/*m*	$\not p$	$\not p$6/*m* (R60)
6/*mmm*	$\not p$	$\not p$6/*mmm* (R73)

(*c*) Frieze groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
2	$\not p$	$\not p$211 (F2)
2*mm*	$\not p$	$\not p$2*mm* (F6)

(ii) If the resulting symmorphic subperiodic group is not centrosymmetric, inversion is added.

There are 13 different Patterson symmetries for the layer groups, ten for the rod groups and two for the frieze groups. These are listed in Table 1.2.5.1. The 'point-group part' of the symbol of the Patterson symmetry represents the *Laue class* to which the subperiodic group belongs (*cf.* Tables 1.2.1.1, 1.2.1.2 and 1.2.1.3).

1.2.6. Subperiodic group diagrams

There are two types of diagrams, referred to as *symmetry diagrams* and *general-position diagrams*. Symmetry diagrams show (i) the relative locations and orientations of the symmetry elements and (ii) the locations and orientations of the symmetry elements relative to a given coordinate system. General-position diagrams show the arrangement of a set of symmetrically equivalent points of general positions relative to the symmetry elements in that given coordinate system.

For the three-dimensional subperiodic groups, *i.e.* layer and rod groups, all diagrams are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system (see Tables 1.2.1.1 and 1.2.1.2). If the other basis vectors are not parallel to the plane of the figure, they are indicated by subscript '*p*', *e.g.* $\mathbf{a}_p$, $\mathbf{b}_p$ and $\mathbf{c}_p$.

For frieze groups (two-dimensional subperiodic groups), the diagrams are in the plane defined by the frieze group's conventional crystallographic coordinate system (see Table 1.2.1.3).

The graphical symbols for symmetry elements used in the symmetry diagrams are given in Chapter 1.1 and follow those used in *IT* A (2005). For rod groups, the 'heights' h along the projection direction above the plane of the diagram are indicated for symmetry planes and symmetry axes *parallel* to the plane of the diagram, for rotoinversions and for centres of symmetry. The heights are given as fractions of the translation along the projection direction and, if different from zero, are printed next to the graphical symbol.

Schematic representations of the diagrams, displaying their conventional coordinate system, *i.e.* the origin and basis vectors, with the basis vectors labelled in the standard setting, are given below. The general-position diagrams are indicated by the letter G.

(i) *Layer groups*

For the layer groups, all diagrams are orthogonal projections along the basis vector **c**. For the triclinic/oblique layer groups, two diagrams are given: the general-position diagram on the right and the symmetry diagram on the left. These diagrams are illustrated in Fig. 1.2.6.1.

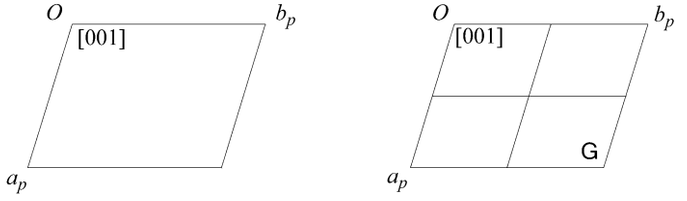

Fig. 1.2.6.1. Diagrams for triclinic/oblique layer groups.

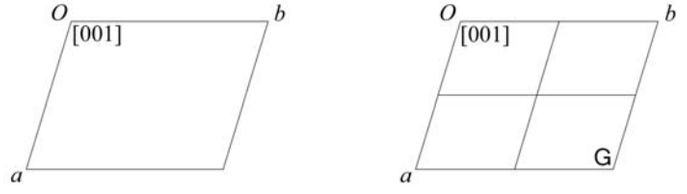

Fig. 1.2.6.2. Diagrams for monoclinic/oblique layer groups.

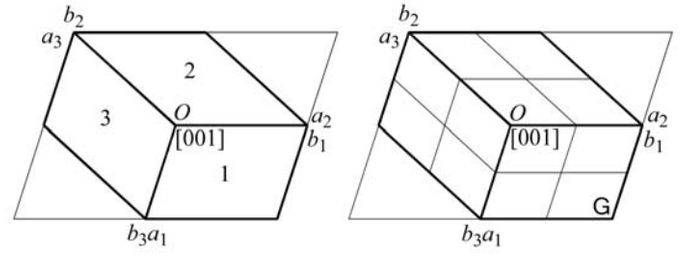

Fig. 1.2.6.3. Monoclinic/oblique layer groups Nos. 5 and 7, cell choices 1, 2, 3. The numbers 1, 2, 3 within the cells and the subscripts of the basis vectors indicate the cell choice.

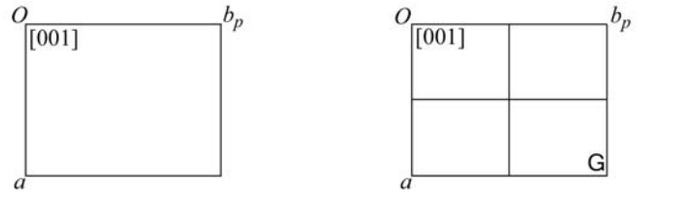

Fig. 1.2.6.4. Diagrams for monoclinic/rectangular layer groups.

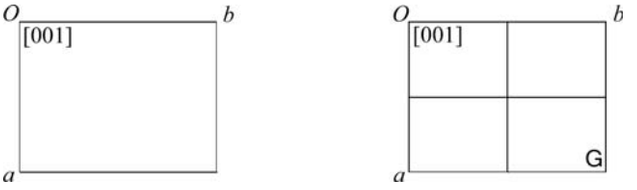

Fig. 1.2.6.5. Diagrams for orthorhombic/rectangular layer groups.

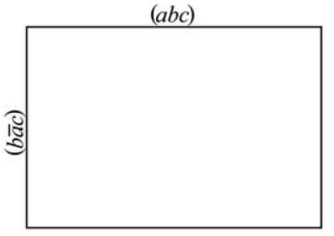

Fig. 1.2.6.6. Monoclinic/rectangular and orthorhombic/rectangular layer groups with two settings. For the second-setting symbol printed vertically, the page must be turned clockwise by 90° or viewed from the right-hand side.

For all monoclinic/oblique layer groups, except groups L5 and L7, two diagrams are given, as shown in Fig. 1.2.6.2. For the layer groups L5 and L7, the descriptions of the three cell choices are headed by a pair of diagrams, as illustrated in Fig. 1.2.6.3. Each diagram is a projection of four neighbouring unit cells. The

Table 1.2.6.1. *Distinct Hermann–Mauguin symbols for monoclinic/rectangular and orthorhombic/rectangular layer groups in different settings*

	Setting symbol	
	(*abc*)	(*bāc*)
Layer group	Hermann–Mauguin symbol	
L8	*p*211	*p*121
L9	$p2_111$	$p12_11$
L10	*c*211	*c*121
L11	*pm*11	*p*1*m*1
L12	*pb*11	*p*1*a*1
L13	*cm*11	*c*1*m*1
L14	*p*2/*m*11	*p*12/*m*1
L15	$p2_1/m11$	$p12_1/m1$
L16	*p*2/*b*11	*p*12/*a*1
L17	$p2_1/b11$	$p12_1/a1$
L18	*c*2/*m*11	*c*12/*m*1
L20	$p2_122$	$p22_12$
L24	*pma*2	*pbm*2
L27	*pm*2*m*	*p*2*mm*
L28	$pm2_1b$	$p2_1ma$
L29	$pb2_1m$	$p2_1am$
L30	*pb*2*b*	*p*2*aa*
L31	*pm*2*a*	*p*2*mb*
L32	$pm2_1n$	$p2_1mn$
L33	$pb2_1a$	$p2_1ab$
L34	*pb*2*n*	*p*2*an*
L35	*cm*2*m*	*c*2*mm*
L36	*cm*2*a*	*c*2*mb*
L38	*pmaa*	*pbmb*
L40	*pmam*	*pbmm*
L41	*pmma*	*pmmb*
L42	*pman*	*pbmn*
L43	*pbaa*	*pbab*
L45	*pbma*	*pmab*

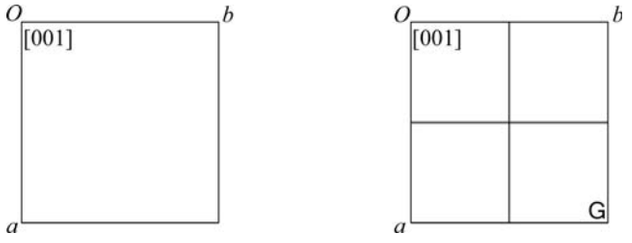

Fig. 1.2.6.7. Diagrams for square/tetragonal layer groups.

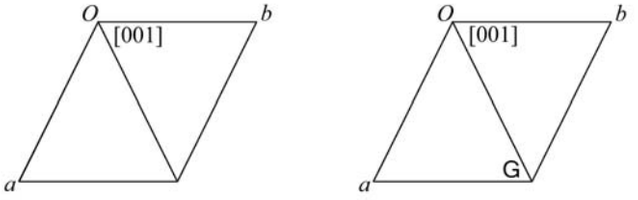

Fig. 1.2.6.8. Diagrams for trigonal/hexagonal and hexagonal/hexagonal layer groups.

headline of each cell choice contains a small drawing indicating the origin and basis vectors of the cell that apply to that description.

For the monoclinic/rectangular and orthorhombic/rectangular layer groups, two diagrams are given, as illustrated in Figs. 1.2.6.4 and 1.2.6.5, respectively. For these groups, the Hermann–Mauguin symbol for the layer group is given for two settings, *i.e.* for two ways of assigning the labels **a**, **b**, **c** to the basis vectors of the conventional coordinate system.

The symbol for each setting is referred to as a *setting symbol*. The setting symbol for the standard setting is (*abc*). The Hermann–Mauguin symbol of the layer group in the conventional coordinate system, in the standard setting, is the same as the Hermann–Mauguin symbol in the first line of the headline. The setting symbol for all other settings is a shorthand notation for the relabelling of the basis vectors. For example, the setting symbol (*cab*) means that the basis vectors relabelled in this setting as **a**, **b** and **c** were in the standard setting labelled **c**, **a** and **b**, respectively [*cf.* Section 2.2.6 of *IT* A (2005)].

For these groups, the two settings considered are the standard (*abc*) setting and a second ($b\bar{a}c$) setting. In Fig. 1.2.6.6, the (*abc*) setting symbol is written horizontally across the top of the diagram and the second ($b\bar{a}c$) setting symbol is written vertically on the left-hand side of the diagram. When viewing the diagram with the (*abc*) setting symbol written horizontally across the top of the diagram, the origin of the coordinate system is at the upper left-hand corner of the diagram, the basis vector labelled **a** is downward towards the bottom of the page, the basis vector labelled **b** is to the right and the basis vector labelled **c** is upward out of the page (see also Figs. 1.2.6.4 and 1.2.6.5). When viewing the diagram with the ($b\bar{a}c$) written horizontally, *i.e.* by rotating the page clockwise by 90° or by viewing the diagram from the right, the position of the origin and the labelling of the basis vectors are as above, *i.e.* the origin is at the upper left-hand corner, the basis vector labelled **a** is downward, the basis vector labelled **b** is to the right and the basis vector labelled **c** is upward out of the page. In the symmetry diagrams of these groups, Part 4, the setting symbols are not given. In their place is given the Hermann–Mauguin symbol of the layer group in the conventional coordinate system in the corresponding setting. The Hermann–Mauguin symbol in the standard setting is given horizontally across the top of the diagram, and in the second setting vertically on the left-hand side.

If the two Hermann–Mauguin symbols are the same (*i.e.* as the Hermann–Mauguin symbol in the first line of the heading), then no symbols are explicitly given. A listing of monoclinic/rectangular and orthorhombic/rectangular layer groups with distinct Hermann–Mauguin symbols in the two settings is given in Table 1.2.6.1.

*Example: The layer group pma*2 *(L24)*

In the (*abc*) setting, the Hermann–Mauguin symbol is *pma*2. In the ($b\bar{a}c$) setting, the Hermann–Mauguin symbol is *pbm*2.

For the square/tetragonal, hexagonal/trigonal and hexagonal/hexagonal layer groups, two diagrams are given, as illustrated in Figs. 1.2.6.7 and 1.2.6.8.

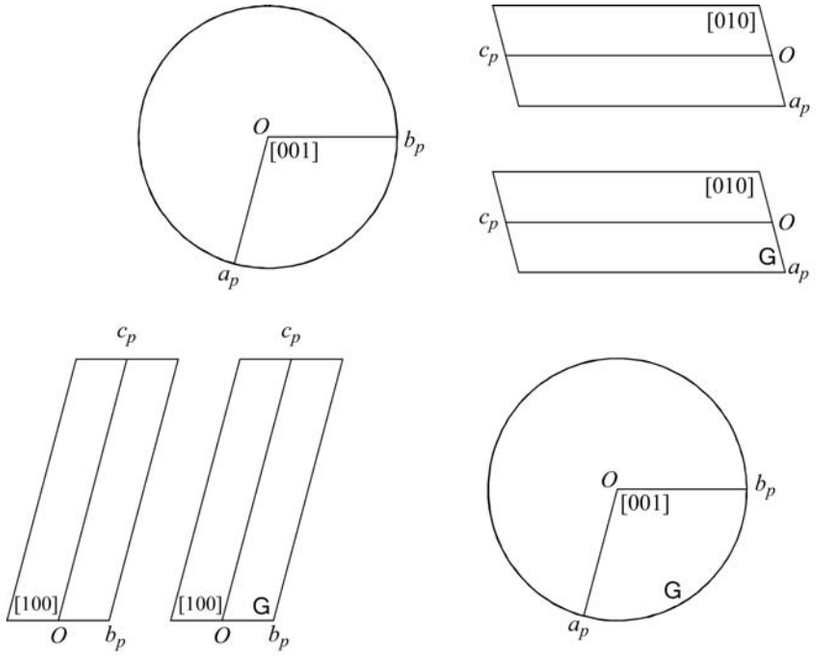

Fig. 1.2.6.9. Diagrams for triclinic rod groups.

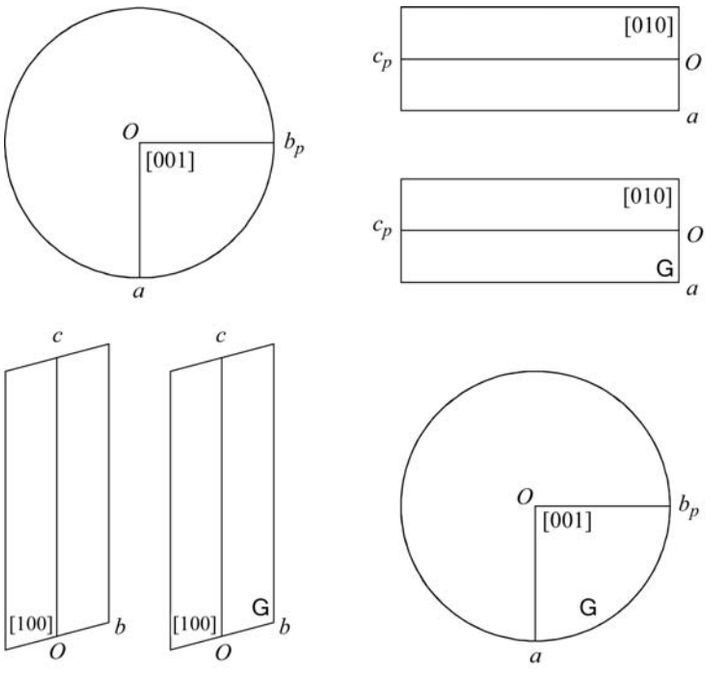

Fig. 1.2.6.10. Diagrams for monoclinic/inclined rod groups.

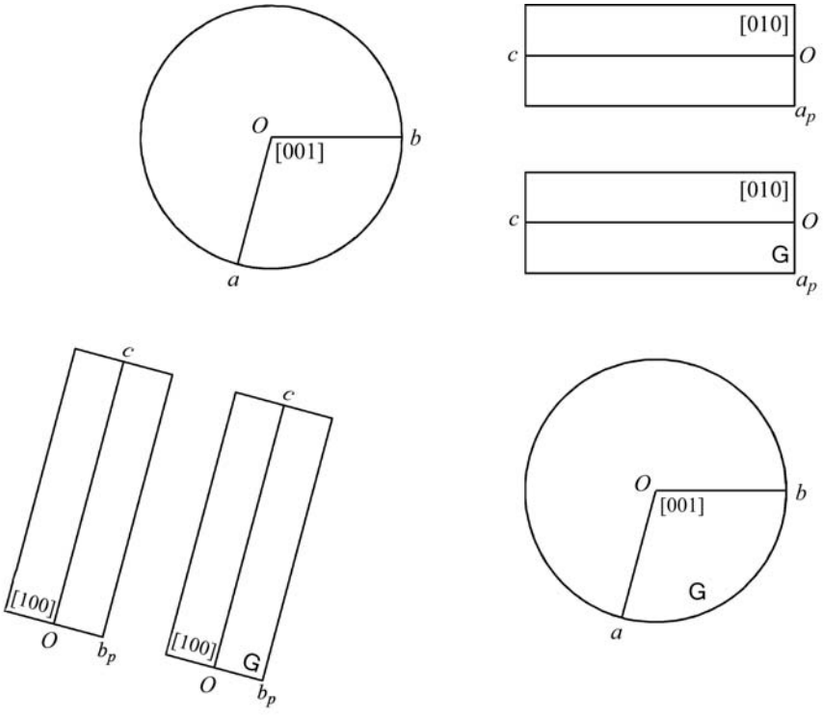

Fig. 1.2.6.11. Diagrams for monoclinic/orthogonal rod groups.

(ii) *Rod groups*

For triclinic, monoclinic/inclined, monoclinic/orthogonal and orthorhombic rod groups, six diagrams are given: three symmetry diagrams and three general-position diagrams. These diagrams are orthogonal projections along each of the conventional coordinate system basis vectors. For pictorial clarity, each of the projections contains an area bounded by a circle or a parallelogram. These areas may be considered as the projections of a cylindrical volume, whose axis coincides with the **c** lattice vector, bounded at $z = 0$ and $z = 1$ by planes parallel to the plane containing the **a** and **b** basis vectors. The projection of the **c** lattice vector is shown explicitly. Only the *directions* of the projected non-lattice basis vectors **a** and **b** are indicated in the diagrams, denoted by lines from the origin to the boundary of the projected cylinder. These diagrams are illustrated for triclinic rod groups in Fig. 1.2.6.9, for monoclinic/inclined rod groups in Fig. 1.2.6.10, for monoclinic/orthogonal rod groups in Fig. 1.2.6.11 and for orthorhombic rod groups in Fig. 1.2.6.12.

The symmetry diagrams consist of the **c** projection, outlined with a circle at the upper left-hand side, the **a** projection at the lower left-hand side and the **b** projection at the upper right-hand side. The general-position diagrams are the **c** projection, outlined with a circle at the lower right-hand side, and the remaining two general-position diagrams next to the corresponding symmetry diagrams.

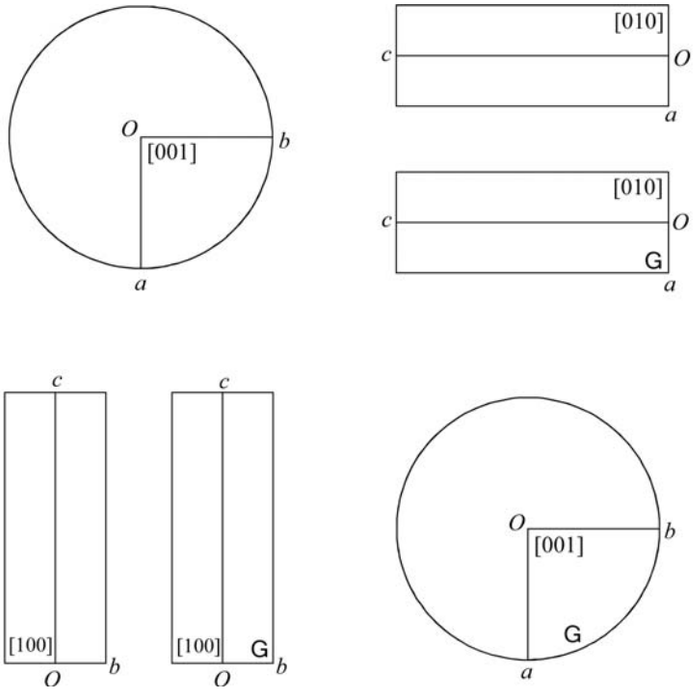

Fig. 1.2.6.12. Diagrams for orthorhombic rod groups.

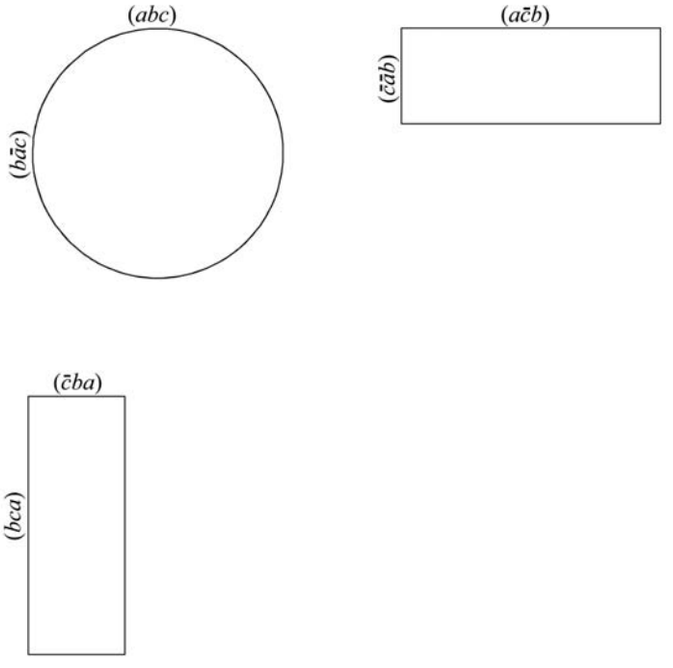

Fig. 1.2.6.13. Setting symbols on symmetry diagrams for the monoclinic/inclined, monoclinic/orthogonal and orthorhombic rod groups.

Six settings for each of these rod groups are considered and the corresponding setting symbols are shown in Fig. 1.2.6.13. This figure schematically shows the three symmetry diagrams each with two setting symbols, one written horizontally across the top of the diagram and the second written vertically along the left-hand side of the diagram. In the symmetry diagrams of these groups, Part 3, the setting symbols are not given. In their place is given the Hermann–Mauguin symbol of the layer group in the conventional coordinate system in the corresponding setting. As there are only translations in one dimension, it is necessary to add

Fig. 1.2.6.14. Diagrams for tetragonal rod groups.

to the translational part of the Hermann–Mauguin symbol a subindex to the lattice symbol to denote the direction of the translations. For example, consider the rod group of the type $\not\!\!\!

Table 1.2.6.2. *Distinct Hermann–Mauguin symbols for monoclinic and orthorhombic rod groups in different settings*

	Setting symbol					
	(abc)	$(b\bar{a}c)$	$(\bar{c}ba)$	(bca)	$(a\bar{c}b)$	$(\bar{c}\bar{a}b)$
Rod group	Hermann–Mauguin symbol					
R3	$\not_c 211$	$\not_c 121$	$\not_a 112$	$\not_b 112$	$\not_b 211$	$\not_a 121$
R4	$\not_c m11$	$\not_c 1m1$	$\not_a 11m$	$\not_b 11m$	$\not_b m11$	$\not_a 1m1$
R5	$\not_c c11$	$\not_c 1c1$	$\not_a 11a$	$\not_b 11b$	$\not_b b11$	$\not_a 1a1$
R6	$\not_c 2/m11$	$\not_c 12/m1$	$\not_a 112/m$	$\not_b 112/m$	$\not_b 2/m11$	$\not_a 12/m1$
R7	$\not_c 2/c11$	$\not_c 12/c1$	$\not_a 112/a$	$\not_b 112/b$	$\not_b 2/b11$	$\not_a 12/a1$
R8	$\not_c 112$	$\not_c 112$	$\not_a 211$	$\not_b 121$	$\not_b 121$	$\not_a 211$
R9	$\not_c 112_1$	$\not_c 112_1$	$\not_a 2_1 11$	$\not_b 12_1 1$	$\not_b 12_1 1$	$\not_a 2_1 11$
R10	$\not_c 11m$	$\not_c 11m$	$\not_a m11$	$\not_b 1m1$	$\not_b 1m1$	$\not_a m11$
R11	$\not_c 112/m$	$\not_c 112/m$	$\not_a 2/m11$	$\not_b 12/m1$	$\not_b 12/m1$	$\not_a 2/m11$
R12	$\not_c 112_1/m$	$\not_c 112_1/m$	$\not_a 2_1/m11$	$\not_b 12_1/m1$	$\not_b 12_1/m1$	$\not_a 2_1/m11$
R13	$\not_c 222$	$\not_c 222$	$\not_a 222$	$\not_b 222$	$\not_b 222$	$\not_a 222$
R14	$\not_c 222_1$	$\not_c 222_1$	$\not_a 2_1 22$	$\not_b 22_1 2$	$\not_b 22_1 2$	$\not_a 2_1 22$
R15	$\not_c mm2$	$\not_c mm2$	$\not_a 2mm$	$\not_b m2m$	$\not_b m2m$	$\not_a 2mm$
R16	$\not_c cc2$	$\not_c cc2$	$\not_a 2aa$	$\not_b b2b$	$\not_b b2b$	$\not_a 2aa$
R17	$\not_c mc2_1$	$\not_c cm2_1$	$\not_a 2_1 am$	$\not_b b2_1 m$	$\not_b m2_1 b$	$\not_a 2_1 ma$
R18	$\not_c 2mm$	$\not_c m2m$	$\not_a mm2$	$\not_b mm2$	$\not_b 2mm$	$\not_a m2m$
R19	$\not_c 2cm$	$\not_c c2m$	$\not_a ma2$	$\not_b bm2$	$\not_b 2mb$	$\not_a m2a$
R20	$\not_c mmm$	$\not_c mmm$	$\not_a mmm$	$\not_b mmm$	$\not_b mmm$	$\not_a mmm$
R21	$\not_c ccm$	$\not_c ccm$	$\not_a maa$	$\not_b bmb$	$\not_b bmb$	$\not_a maa$
R22	$\not_c mcm$	$\not_c cmm$	$\not_a mam$	$\not_b bmm$	$\not_b mmb$	$\not_a mma$

Table 1.2.6.3. *Distinct Hermann–Mauguin symbols for tetragonal, trigonal and hexagonal rod groups in different settings*

	Setting symbol	
	(abc)	$(a \pm b \quad b \mp a \quad c)$
Rod group	Hermann–Mauguin symbol	
R35	$\not_4 2_1 cm$	$\not_4 2_1 mc$
R37	$\not_{\bar{4}} 2m$	$\not_{\bar{4}} m2$
R38	$\not_{\bar{4}} 2c$	$\not_{\bar{4}} c2$
R41	$\not_4 2_1/mmc$	$\not_4 2_1/mcm$

	Setting symbol	
	(abc)	$(\pm 2a \pm b \quad \mp a \pm b \quad c)$ $(\pm a \pm 2b \quad \mp 2a \mp b \quad c)$ $(\mp a \pm b \quad \mp a \mp 2b \quad c)$
Rod group	Hermann–Mauguin symbol	
R46	$\not_3 12$	$\not_3 21$
R47	$\not_3 1_1 2$	$\not_3 1_1 21$
R48	$\not_3 1_2 2$	$\not_3 2_1 21$
R49	$\not_3 m1$	$\not_3 1m$
R50	$\not_3 c1$	$\not_3 1c$
R51	$\not_{\bar{3}} 1m$	$\not_{\bar{3}} m1$
R52	$\not_{\bar{3}} 1c$	$\not_{\bar{3}} c1$
R70	$\not_6 3mc$	$\not_6 3cm$
R71	$\not_{\bar{6}} m2$	$\not_{\bar{6}} 2m$
R72	$\not_{\bar{6}} c2$	$\not_{\bar{6}} 2c$
R75	$\not_6 3/mmc$	$\not_6 3/mcm$

position diagram. These diagrams are illustrated in Figs. 1.2.6.14 and 1.2.6.15. One can consider additional settings for these rod groups: see the setting symbols in Table 1.2.6.3. If the Hermann–Mauguin symbols for the group in these settings are identical, only one tabulation of the group, in the standard setting, is given. If in these settings two distinct Hermann–Mauguin symbols are obtained, a second tabulation for the rod group is given. This second tabulation is in the conventional coordinate system in the $(a+b \quad \overline{a}+b \quad c)$ setting for tetragonal groups, and in the

Fig. 1.2.6.15. Diagrams for trigonal and hexagonal rod groups.

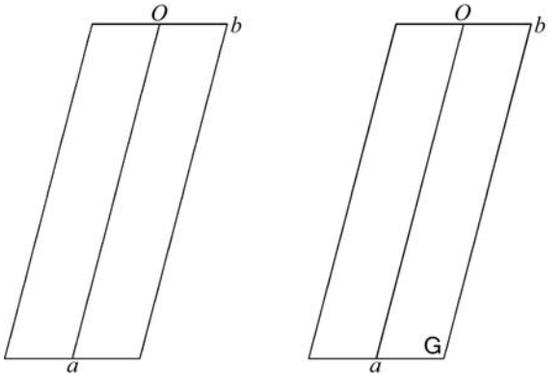

Fig. 1.2.6.16. Diagrams for oblique frieze groups.

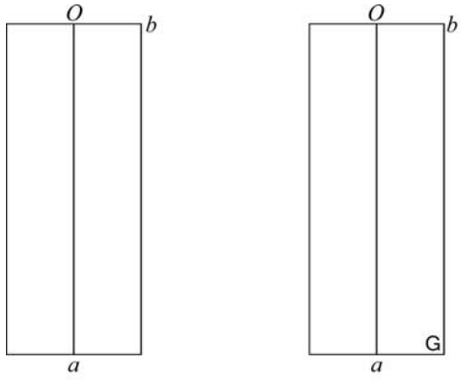

Fig. 1.2.6.17. Diagrams for rectangular frieze groups.

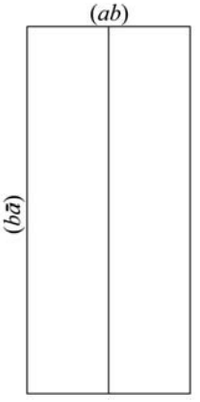

Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

$(2a+b\ \ \bar{a}+b\ \ c)$ setting for trigonal and hexagonal groups. These second tabulations aid in the correlation of Wyckoff positions of space groups and Wyckoff positions of rod groups. For example, the Wyckoff positions of the two space groups types $P3m1$ and $P31m$ can be easily correlated with, respectively, the Wyckoff positions of a rod group of the type R49 in the standard setting where the Hermann–Mauguin symbol is $\not3m1$ and in the second setting where the symbol is $\not31m$. In Table 1.2.6.3, we list the tetragonal, trigonal and hexagonal rod groups where in the different settings the two Hermann–Mauguin symbols are distinct.

(iii) *Frieze groups*

Two diagrams are given for each frieze group: a symmetry diagram and a general-position diagram. These diagrams are illustrated for the oblique and rectangular frieze groups in Figs. 1.2.6.16 and 1.2.6.17, respectively. We consider the two settings (ab) and $(b\bar{a})$, see Fig. 1.2.6.18. In the frieze-group tables, Part 2, we replace the setting symbols with the corresponding Hermann–Mauguin symbols where a subindex is added to the lattice symbol to denote the direction of the translations. A listing of the frieze groups with the Hermann–Mauguin symbols of each group in the two settings is given in Table 1.2.6.4.

Table 1.2.6.4. *Distinct Hermann–Mauguin symbols for frieze groups in different settings*

	Setting symbol	
	(ab)	$(b\bar{a})$
Frieze group	Hermann–Mauguin symbol	
F1	$\not_a1$	$\not_b1$
F2	$\not_a211$	$\not_b211$
F3	$\not_a1m1$	$\not_b11m$
F4	$\not_a11m$	$\not_b1m1$
F5	$\not_a11g$	$\not_b1g1$
F6	$\not_a2mm$	$\not_b2mm$
F7	$\not_a2mg$	$\not_b2gm$

1.2.7. Origin

The origin has been chosen according to the following conventions:

(i) If the subperiodic group is centrosymmetric, then the inversion centre is chosen as the origin. For the three layer groups $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (L64), we give descriptions for two origins, at the inversion centre and at $(-\frac{1}{4},-\frac{1}{4},0)$ from the inversion centre. This latter origin is at a position of high site symmetry and is consistent with having the origin on the fourfold axis, as is the case for all other tetragonal layer groups. The group symbols for the description with the origin at the inversion centre, *e.g.* $p4/n(\frac{1}{4},\frac{1}{4},0)$, are followed by the shift $(\frac{1}{4},\frac{1}{4},0)$ of the position of the origin used in the description having the origin on the fourfold axis.

(ii) For noncentrosymmetric subperiodic groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetry elements.

Origin statement: In the line *Origin* immediately below the diagrams, the site symmetry of the origin is stated if different from the identity. A further symbol indicates all symmetry elements that pass through the origin. For the three layer groups $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (L64) where the origin is on the fourfold axis, the statement 'at $-\frac{1}{4},-\frac{1}{4},0$ from centre' is given to denote the position of the origin with respect to an inversion centre.

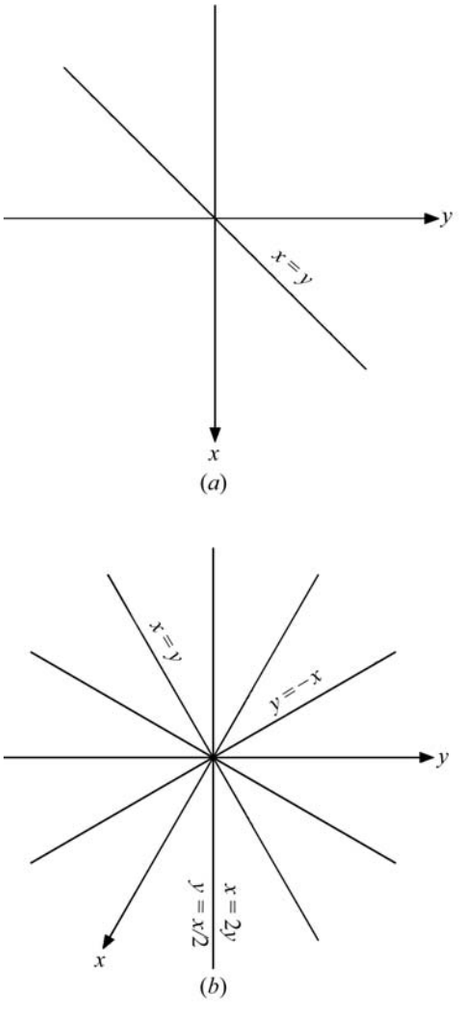

Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (*a*) tetragonal rod groups and (*b*) trigonal and hexagonal rod groups.

1.2.8. Asymmetric unit

An asymmetric unit of a subperiodic group is a simply connected smallest part of space from which, by application of all symmetry operations of the subperiodic group, the whole space is filled exactly. For three-dimensional (two-dimensional) space groups,

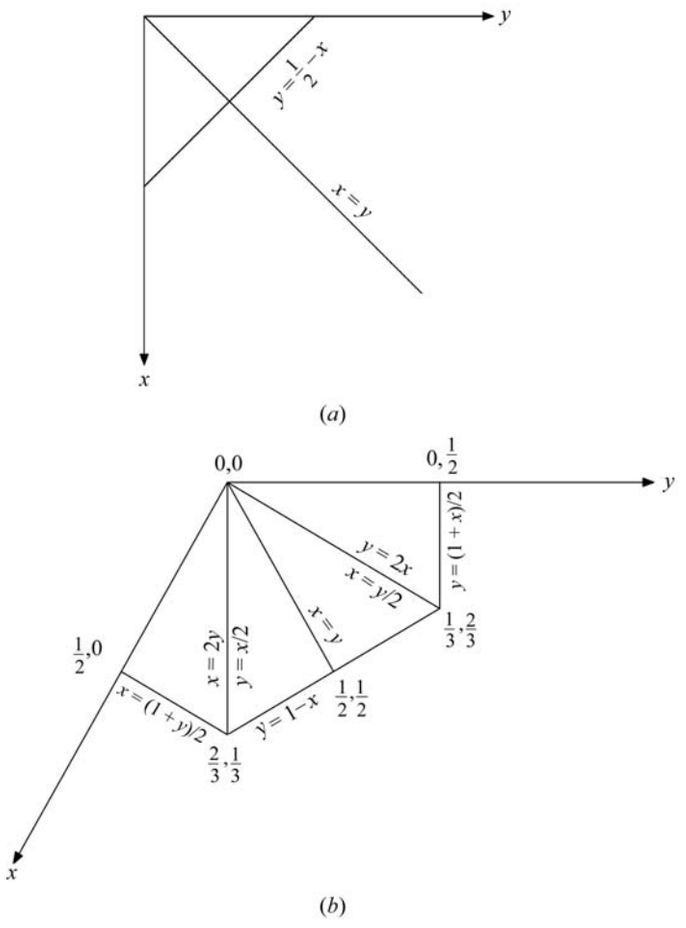

Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (*a*) tetragonal/square layer groups and (*b*) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (*b*), the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are also given.

because they contain three-dimensional (two-dimensional) translational symmetry, the asymmetric unit is a finite part of space [see Section 2.2.8 of *IT* A (2005)]. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. We define the asymmetric unit for subperiodic groups by setting the limits on the coordinates of points contained in the asymmetric unit.

1.2.8.1. Frieze groups

For all frieze groups, a limit is set on the x coordinate of the asymmetric unit by the inequality

$$0 \le x \le \text{ upper limit on } x.$$

For the y coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero, *i.e.* $0 \le y$.

Example: The frieze group $\not{p}2mm$ (F6)

Asymmetric unit $0 \le x \le 1/2;\ 0 \le y.$

1.2.8.2. Rod groups

For all rod groups, a limit is set on the z coordinate of the asymmetric unit by the inequality

$$0 \le z \le \text{ upper limit on } z.$$

For each of the x and y coordinates, either there is no limit and nothing further is written, or there is the lower limit of zero.

For tetragonal, trigonal and hexagonal rod groups, additional limits are required to define the asymmetric unit. These limits are given by additional inequalities, such as $x \le y$ and $y \le x/2$. Fig. 1.2.8.1 schematically shows the boundaries represented by such inequalities.

Example: The rod group $\not{p}6_3mc$ (R70)

Asymmetric unit $0 \le x;\ 0 \le y;\ 0 \le z \le 1;\ y \le x/2.$

1.2.8.3. Layer groups

For all layer groups, limits are set on the x coordinate and y coordinate of the asymmetric unit by the inequalities

$$0 \le x \le \text{ upper limit on } x$$
$$0 \le y \le \text{ upper limit on } y.$$

For the z coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero.

For tetragonal/square, trigonal/hexagonal and hexagonal/hexagonal layer groups, additional limits are required to define the asymmetric unit. These additional limits are given by additional inequalities. Fig. 1.2.8.2 schematically shows the boundaries represented by these inequalities. For trigonal/hexagonal and hexagonal/hexagonal layer groups, because of the complicated shape of the asymmetric unit, the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are given.

Example: The layer group p3m1 (L69)

Asymmetric unit $0 \le x \le 2/3;\ 0 \le y \le 2/3;\ x \le 2y;$
$y \le \min(1 - x, 2x)$

Vertices $0, 0;\ 2/3, 1/3;\ 1/3, 2/3.$

1.2.9. Symmetry operations

The coordinate triplets of the *General position* of a subperiodic group may be interpreted as a shorthand description of the symmetry operations in matrix notation as in the case of space groups [see Sections 2.2.3, 8.1.5 and 11.1.1 of *IT* A (2005)]. The geometric description of the symmetry operations is found in the subperiodic group tables under the heading *Symmetry operations*. These data form a link between the subperiodic group diagrams (Section 1.2.6) and the general position (Section 1.2.11). Below the geometric description we give the Seitz notation (Burns & Glazer, 1990) of each symmetry operation using the subindex notation of Zak *et al.* (1969).

1.2.9.1. Numbering scheme

The numbering (1) ... (p) ... of the entries in the blocks *Symmetry operations* and *General position* (first block below *Positions*) is the same. Each listed coordinate triplet of the general position is preceded by a number between parentheses (p). The same number (p) precedes the corresponding symmetry operation. For all subperiodic groups with *primitive* lattices, the two lists contain the same number of entries.

For the nine layer groups with *centred* lattices, to the one block of *General positions* correspond two blocks of *Symmetry operations*. The numbering scheme is applied to both blocks. The two blocks correspond to the two centring translations below the subheading *Coordinates*, *i.e.* $(0, 0, 0)+ \quad (1/2, 1/2, 0)+$. For the *Positions*, the reader is expected to add these two centring

translations to each printed coordinate triplet in order to obtain the complete general position. For the *Symmetry operations*, the corresponding data are listed explicitly with the two blocks having the subheadings 'For (0, 0, 0)+ set' and 'For (1/2, 1/2, 0)+ set', respectively.

1.2.9.2. Designation of symmetry operations

The designation of symmetry operations for the subperiodic groups is the same as for the space groups. An entry in the block *Symmetry operations* is characterized as follows:

(i) A symbol denoting the *type* of the symmetry operation [*cf.* Chapter 1.2 of *IT* A (2005)], including its glide or screw part, if present. In most cases, the glide or screw part is given explicitly by fractional coordinates between parentheses. The sense of a rotation is indicated by the superscript + or −. Abbreviated notations are used for the glide reflections $a(1/2,\ 0,\ 0) \equiv a$; $b(0, 1/2, 0) \equiv b$; $c(0, 0, 1/2) \equiv c$. Glide reflections with complicated and unconventional glide parts are designated by the letter *g*, followed by the glide part between parentheses.

(ii) A coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation. For rotoinversions the location of the inversion point is also given.

Details of this symbolism are given in Section 11.1.2 of *IT* A (2005).

Examples

(1) $m \quad x, 0, z$: a reflection through the plane $x, 0, z$, *i.e.* the plane parallel to (010) containing the point (0, 0, 0).

(2) $m \quad x + 1/2, \bar{x}, z$: a reflection through the plane $x + 1/2, \bar{x}, z$, *i.e.* the plane parallel to (110) containing the point (1/2, 0, 0).

(3) $g(1/2, 1/2, 0) \quad x, x, z$: glide reflection with glide component (1/2, 1/2, 0) through the plane x, x, z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point (0, 0, 0).

(4) $2(1/2, 0, 0) \quad x, 1/4, 0$: screw rotation along the (100) direction containing the point (0, 1/4, 0) with a screw component (1/2, 0, 0).

(5) $\bar{4}^- \quad 1/2, 0, z \quad 1/2, 0, 0$: fourfold rotoinversion consisting of a clockwise rotation by 90° around the line $1/2, 0, z$ followed by an inversion through the point (1/2, 0, 0).

1.2.10. Generators

The line *Generators selected* states the symmetry operations and their sequence selected to generate all symmetrically equivalent points of the *General position* from a point with coordinates x, y, z. The identity operation given by (1) is always selected as the first generator. The generating translations are listed next, $t(1, 0)$ for frieze groups, $t(0, 0, 1)$ for rod groups, and $t(1, 0, 0)$ and $t(0, 1, 0)$ for layer groups. For centred layer groups, there is the additional centring translation $t(1/2, 1/2, 0)$. The additional generators are given as numbers (p) which refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*; for centred layer groups, the first block 'For (0, 0, 0)+ set' must be used.

1.2.11. Positions

The entries under *Positions* (more explicitly called *Wyckoff positions*) consist of the *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity M* of the Wyckoff position. This is the number of equivalent points per conventional cell. The multiplicity *M* of the general position is equal to the order of the point group of the subperiodic group, except in the case of centred layer groups when it is twice the order of the point group. The multiplicity *M* of a special position is equal to the order of the point group of the subperiodic group divided by the order of the site-symmetry group (see Section 1.2.12).

(ii) *Wyckoff letter*. This letter is a coding scheme for the Wyckoff positions, starting with *a* at the bottom position and continuing upwards in alphabetical order.

(iii) *Site symmetry*. This is explained in Section 1.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators*. For the centred layer groups, the centring translations (0, 0, 0)+ and (1/2, 1/2, 0)+ are listed above the coordinate triplets. The symbol '+' indicates that in order to obtain a complete Wyckoff position, the components of these centring translations have to be added to the listed coordinate triplets.

(v) *Reflection conditions*. These are described in Section 1.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*. A set of symmetrically equivalent points is said to be in a 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the subperiodic group.

(ii) *Special position(s)*. A set of symmetrically equivalent points is said to be in a 'special position' if each of its points is mapped onto itself by at least one additional operation in addition to the identity operation.

Example: Layer group c2/m11 (L18)

The general position 8*f* of this layer group contains eight equivalent points per cell each with site symmetry 1. The coordinate triplets of four points (1) to (4) are given explicitly, the coordinate triplets of the other four points are obtained by adding the components (1/2, 1/2, 0) of the *c*-centring translation to the coordinate triplets (1) to (4).

This layer group has five special positions with the Wyckoff letters *a* to *e*. The product of the multiplicity and the order of the site-symmetry group is the multiplicity of the general position. For position 4*d*, for example, the four equivalent points have the coordinates $x, 0, 0$, $\bar{x}, 0, 0$, $x + 1/2, 1/2, 0$ and $\bar{x} + 1/2, 1/2, 0$. Since each point of position 4*d* is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from eight to four, whereas the order of the site symmetry is increased from one to two.

1.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *site symmetry* of that position. The site-symmetry group is isomorphic to a proper or improper subgroup of the point group to which the subperiodic group under consideration belongs. *Oriented site-symmetry symbols* are used to show how the symmetry elements at a site are related to the conventional crystallographic basis. The site-symmetry symbols display the same sequence of symmetry directions as the subperiodic group symbol (*cf.* Table 1.2.4.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. Sets of symmetry directions having more than one equivalent direction may require more than one character if

Table 1.2.13.1. *General reflection conditions due to glide planes and screw axes*

(*a*) Layer groups.
(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
hk: $h = 2n$	(001)	**a**/2	*a*
hk: $k = 2n$	(001)	**b**/2	*b*
hk: $h + k = 2n$	(001)	**a**/2 + **b**/2	*n*
$0k$: $k = 2n$	(100)	**b**/2	*b*
$h0$: $h = 2n$	(010)	**a**/2	*a*

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$h0$: $h = 2n$	[100]	**a**/2	2_1
$0k$: $k = 2n$	[010]	**b**/2	2_1

(*b*) Rod groups.
(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
l: $l = 2n$	Any orientation parallel to the *c* axis	**c**/2	*c*

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
l: $l = 2n$	[001]	**c**/2	2_1, 4_2, 6_3
l: $l = 3n$	[001]	**c**/3	3_1, 3_2, 6_2, 6_4
l: $l = 4n$	[001]	**c**/4	4_1, 4_3
l: $l = 6n$	[001]	**c**/6	6_1, 6_5

(*c*) Frieze groups, glide plane.

Reflection condition	Orientation of plane	Glide vector	Symbol
h: $h = 2n$	(10)	**a**/2	*g*

the site-symmetry group belongs to a lower crystal system. For example, for the 2*c* position of tetragonal layer group *p*4*mm* (L55), the site-symmetry group is the orthorhombic group '2*mm*.'. The two characters '*mm*' represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry direction.

1.2.13. Reflection conditions

The *Reflection conditions* are listed in the right-hand column of each Wyckoff position. There are two types of reflection conditions:

(i) *General conditions*. These conditions apply to *all* Wyckoff positions of the subperiodic group.

(ii) *Special conditions* ('extra' conditions). These conditions apply only to *special* Wyckoff positions and must always be added to the general conditions of the subperiodic group.

The *general reflection conditions* are the result of three effects: centred lattices, glide planes and screw axes. For the nine layer groups with *centred* lattices, the corresponding general reflection condition is $h + k = 2n$. The general reflection conditions due to glide planes and screw axes for the subperiodic groups are given in Table 1.2.13.1.

*Example: The layer group p*4*bm (L56)*

General position 8*d*: $0k\colon k = 2n$ and $h0\colon h = 2n$ due respectively to the glide planes *b* and *a*. The projections along [100] and [010] of any crystal structure with this layer-group symmetry have, respectively, periodicity **b**/2 and **a**/2.

Special positions 2*a* and 2*b*: $hk\colon h + k = 2n$. Any set of equivalent atoms in either of these positions displays additional *c*-centring.

1.2.14. Symmetry of special projections

1.2.14.1. Data listed in the subperiodic group tables

Under the heading *Symmetry of special projections*, the following data are listed for three orthogonal projections of each layer group and rod group and two orthogonal projections of each frieze group:

(i) For layer and rod groups, each projection is made onto a plane normal to the projection direction. If there are three kinds of symmetry directions (*cf.* Table 1.2.4.1), the three projection directions correspond to the primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction(s) are taken along coordinate axes.

For frieze groups, each projection is made on a line normal to the projection direction.

The directions for which data are listed are as follows:

(*a*) *Layer groups*:

Triclinic/oblique Monoclinic/oblique Monoclinic/rectangular Orthorhombic/rectangular	[001], [100], [010]
Tetragonal/square	[001], [100], [110]
Trigonal/hexagonal Hexagonal/hexagonal	[001], [100], [210]

(*b*) *Rod groups*:

Triclinic Monoclinic/inclined Monoclinic/orthogonal Orthorhombic	[001], [100], [010]
Tetragonal	[001], [100], [110]
Trigonal Hexagonal	[001], [100], [210]

(*c*) *Frieze groups*:

Oblique Rectangular	[10], [01]

(ii) *The Hermann–Mauguin symbol*. For the [001] projection of a layer group, the Hermann–Mauguin symbol for the plane group resulting from the projection of the layer group is given. For the [001] projection of a rod group, the Hermann–Mauguin symbol for the resulting two-dimensional point group is given. For the remainder of the projections, in the case of both layer groups and

Table 1.2.14.1. *a′, b′, γ′ (a′) of the projected conventional coordinate system in terms of a, b, c, α, β, γ (a, b, γ) of the conventional coordinate system of the layer and rod groups (frieze groups)*

(*a*) Layer groups.

Projection direction	Triclinic/oblique	Monoclinic/oblique
[001]	$a' = a \sin\beta$ $b' = b \sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a$ $b' = b$ $\gamma' = \gamma$
[100]	$a' = b \sin\gamma$ $b' = c \sin\beta$ $\gamma' = 180^\circ - \alpha^*$†	$a' = b \sin\gamma$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a \sin\gamma$ $b' = c \sin\alpha$ $\gamma' = 180^\circ - \beta^*$†	$a' = a \sin\gamma$ $b' = c$ $\gamma' = 90^\circ$
	Monoclinic/ rectangular	Orthorhombic/ rectangular
[001]	$a' = a$ $b' = b \sin\alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b$ $b' = c$ $\gamma' = \alpha$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a$ $b' = c \sin\alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = c$ $\gamma' = 90^\circ$
	Tetragonal/square	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = a$ $b' = c$ $\gamma' = 90^\circ$	
[110]	$a' = (a/2)(2)^{1/2}$ $b' = c$ $\gamma' = 90^\circ$	
	Trigonal/hexagonal, hexagonal/hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = [(3)^{1/2}/2]a$ $b' = c$ $\gamma' = 90^\circ$	
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90^\circ$	

† $\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/(\sin\beta\sin\gamma)$,
$\cos\beta^* = (\cos\gamma\cos\alpha - \cos\beta)/(\sin\gamma\sin\alpha)$,
$\cos\gamma^* = (\cos\alpha\cos\beta - \cos\gamma)/(\sin\alpha\sin\beta)$.

(*b*) Rod groups.

Projection direction	Triclinic	Monoclinic/inclined
[001]	$a' = a \sin\beta$ $b' = b \sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a$ $b' = b \sin\alpha$ $\gamma' = 90^\circ$
[100]	$a' = c \sin\beta$ $b' = b \sin\gamma$ $\gamma' = 180^\circ - \alpha^*$†	$a' = c$ $b' = b$ $\gamma = \alpha$
[010]	$a' = c \sin\alpha$ $b' = a \sin\gamma$ $\gamma' = 180^\circ - \beta^*$†	$a' = c \sin\alpha$ $b' = a$ $\gamma' = 90^\circ$
	Monoclinic/ orthogonal	Orthorhombic
[001]	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = c$ $b' = b \sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = b$ $\gamma' = 90^\circ$
[010]	$a' = c$ $b' = a \sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$
	Tetragonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = c$ $b' = a$ $\gamma' = 90^\circ$	
[110]	$a' = c$ $b' = (a/2)(2)^{1/2}$ $\gamma' = 90^\circ$	
	Trigonal, hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = c$ $b' = [(3)^{1/2}/2]a$ $\gamma' = 90^\circ$	
[210]	$a' = c$ $b' = a/2$ $\gamma' = 90^\circ$	

(*c*) Frieze groups.

Projection direction	Oblique	Rectangular
[10]	$a' = b \sin\gamma$	$a' = b$
[01]	$a' = a \sin\gamma$	$a' = a$

rod groups, the Hermann–Mauguin symbol is given for the resulting frieze group. For the [10] projection of a frieze group, the Hermann–Mauguin symbol of the resulting one-dimensional point group, *i.e.* 1 or *m*, is given. For the [01] projection, the Hermann–Mauguin symbol of the resulting one-dimensional space group, *i.e.* *p*1 or *pm*, is given.

(iii) For layer groups, the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ of the plane group resulting from the [001] projection and the basis vector $\mathbf{a}'$ of the frieze groups resulting from the additional two projections are given as linear combinations of the basis vectors **a**, **b** of the layer group. Basis vectors **a**, **b** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$. For the two projections of a rod group resulting in a frieze group, the basis vector $\mathbf{a}'$ of the resulting frieze group is given in terms of the basis vector **c** of the rod group. For the [01] projection of a frieze group, the basis vector $\mathbf{a}'$ of the resulting one-dimensional space group is given in terms of the basis vector **a** of the frieze group.

For rod groups and layer groups, the relations between a', b' and γ' of the projected conventional basis vectors and a, b, c, α, β and γ of the conventional basis vectors of the subperiodic group are given in Table 1.2.14.1. We also give in this table the relations between a' of the projected conventional basis and a, b and γ of the conventional basis of the frieze group.

Table 1.2.14.2. *Projection of three-dimensional symmetry elements (layer and rod groups)*

Symmetry element in three dimensions		Symmetry element in projection	
Arbitrary orientation			
Symmetry centre $\bar{1}$		Rotation point 2 at projection of centre	
Parallel to projection direction			
Rotation axis	2, 3, 4, 6	Rotation point	2, 3, 4, 6
Screw axis	2_1	Rotation point	2
	3_1, 3_2		3
	4_1, 4_2, 4_3		4
	6_1, 6_2, 6_3, 6_4, 6_5		6
Rotoinversion axis	$\bar{4}$	Rotation point	4
	$\bar{6} \equiv 3/m$		3 (with overlap of atoms)
	$\bar{3} \equiv 3 \times \bar{1}$		6
Reflection plane m		Reflection line m	
Glide plane with $\perp$ component†		Glide line g	
Glide plane without $\perp$ component†		Reflection line m	
Normal to projection direction			
Rotation axis	2, 4, 6	Reflection line m	
	3	None	
Screw axis	4_2, 6_2, 6_4	Reflection line m	
	2_1, 4_1, 4_3, 6_1, 6_3, 6_5	Glide line g	
	3_1, 3_2	None	
Rotoinversion axis	$\bar{4}$	Reflection line m parallel to axis	
	$\bar{6} \equiv 3/m$	Reflection line m perpendicular to axis	
	$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)	
Reflection plane m		None, but overlap of atoms	
Glide plane with glide component **t**		Translation **t**	

† The term 'with $\perp$ component' refers to the component of the glide vector normal to the projection direction.

(iv) *Location of the origin* of the plane group, frieze group and one-dimensional space group is given with respect to the conventional lattice of the subperiodic group. The same description is used as for the location of symmetry elements (see Section 1.2.9). *Example*: 'Origin at x, 0, 0' or 'Origin at x, 1/4, 0'.

1.2.14.2. Projections of centred subperiodic groups

The only centred subperiodic groups are the nine types of centred layer groups. For the [100] and [010] projection directions, because of the centred layer-group lattice, the basis vectors of the resulting frieze groups are $\mathbf{a}' = \mathbf{b}/2$ and $\mathbf{a}' = \mathbf{a}/2$, respectively.

1.2.14.3. Projection of symmetry elements

A symmetry element of a subperiodic group projects as a symmetry element only if its orientation bears a special relationship to the projection direction. In Table 1.2.14.2, the three-dimensional symmetry elements of the layer and rod groups and in Table 1.2.14.3 the two-dimensional symmetry elements of the frieze groups are listed along with the corresponding symmetry element in projection.

Example: Layer group cm2m (L35)

Projection along [001]: This orthorhombic/rectangular plane group is centred; m perpendicular to [100] is projected as a reflection line, 2 parallel to [010] is projected as the same reflection line and m perpendicular to [001] gives rise to no symmetry element in projection, but to an overlap of atoms. *Result*: Plane group $c1m1$ (5) with $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$.

Projection along [100]: The frieze group has the basis vector $\mathbf{a}' = \mathbf{b}/2$ due to the centred lattice of the layer group. m perpendicular to [100] gives rise only to an overlap of atoms, 2 parallel to [010] is projected as a reflection line and m perpendicular to [001] is projected as the same reflection line. *Result*: Frieze group $\not\!\!\!

Table 1.2.14.3. *Projection of two-dimensional symmetry elements (frieze groups)*

Symmetry element in two dimensions	Symmetry element in projection
Rotation point 2	Reflection point *m*
Parallel to projection direction	
Reflection line *m* Glide line *g*	Reflection point *m* Reflection point *m*
Normal to projection direction	
Reflection line *m* Glide line *g* with glide component **t**	None (with overlap of atoms) Translation **t**

(iii) minimal non-isotypic non-enantiomorphic supergroups and

(iv) minimal isotypic supergroups and enantiomorphic supergroups of lowest index,

where *isotypic* means 'belonging to the same subperiodic group type'. The cases of maximal enantiomorphic subgroups of lowest index and minimal enantiomorphic supergroups of lowest index arise only in the case of rod groups.

1.2.15.1. Maximal non-isotypic non-enantiomorphic subgroups

The maximal non-isotypic non-enantiomorphic subgroups **S** of a subperiodic group **G** are divided into two types:

I *translationengleiche* or *t* subgroups and

II *klassengleiche* or *k* subgroups.

Type **II** is subdivided again into two blocks:

IIa: the conventional cells of **G** and **S** are the same, and

IIb: the conventional cell of **S** is larger than that of **G**.

Block **IIa** has no entries for subperiodic groups with a primitive cell. Only in the case of the nine centred layer groups are there entries, when it contains those maximal subgroups **S** which have lost all the centring translations of **G** but none of the integral translations.

*1.2.15.1.1. Blocks **I** and **IIa***

In blocks **I** and **IIa**, *every* maximal subgroup **S** of a subperiodic group **G** is listed with the following information:

[*i*] HMS1 (HMS2) Sequence of numbers

The symbols have the following meaning:

[*i*]: index of **S** in **G**.

HMS1: short Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(HMS2): conventional short Hermann–Mauguin symbol of **S**, given only if HMS1 is not in conventional short form.

Sequence of numbers: coordinate triplets of **G** retained in **S**. The numbers refer to the numbering scheme of the coordinate triplets of the general position. For the centred layer groups the following abbreviations are used:

Block **I** (all translations retained). *Number* +: coordinate triplet given by *Number*, plus that obtained by adding the centring translation (1/2, 1/2, 0) of **G**. (*Numbers*) +: the same as above, but applied to all *Numbers* between parentheses.

Block **IIa** (not all translations retained). *Number* + (1/2, 1/2, 0): coordinate triplet obtained by adding the translation (1/2, 1/2, 0) to the triplet given by *Number*. (*Numbers*) + (1/2, 1/2, 0): the same as above, but applied to all *Numbers* between parentheses.

Examples

(1) **G**: Layer group $c211$ (L10)

I	[2]	$c1\,(p1)$	$1+$
IIa	[2]	$p2_111$	$1; 2 + (1/2, 1/2, 0)$
	[2]	$p211$	$1; 2$

where the numbers have the following meaning:

$1+$	x, y, z	$x + 1/2, y + 1/2, z$
$1; 2$	x, y, z	$x, \bar{y}, \bar{z}$
$1; 2+$	x, y, z	$x + 1/2, \bar{y} + 1/2, \bar{z}$

(2) **G**: Rod group $\not p422$ (R30)

I	[2]	$\not p411\,(\not p4)$	$1; 2; 3; 4$
	[2]	$\not p221\,(\not p222)$	$1; 2; 5; 6$
	[2]	$\not p212\,(\not p222)$	$1; 2; 7; 8$

The HMS1 symbol in each of the three subgroups **S** is given in the tetragonal coordinate system of the group **G**. In the first case, $\not p411$ is not the conventional short Hermann–Mauguin symbol and a second conventional symbol $\not p4$ is given. In the latter two cases, since the subgroups are orthorhombic rod groups, a second conventional symbol of the subgroup in an orthorhombic coordinate system is given.

*1.2.15.1.2. Block **IIb***

Whereas in blocks **I** and **IIa** *every* maximal subgroup **S** of **G** is listed, *this is no longer the case* for the entries of block **IIb**. The information given in this block is

[*i*] HMS1 (Vectors) (HMS2)

The symbols have the following meaning:

[*i*]: index of **S** in **G**.

HMS1: Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(Vectors): basis vectors of **S** in terms of the basis vectors of **G**. No relations are given for basis vectors which are unchanged.

(HMS2): conventional short Hermann–Mauguin symbol, given only if HMS1 is not in conventional short form.

Examples

(1) **G**: Rod group $\not p222$ (R13)

IIb [2] $\not p222_1$ ($\mathbf{c}' = 2\mathbf{c}$)

There are two subgroups which obey the same basis-vector relation. Apart from the translations of the enlarged cell, the generators of the subgroups, referred to the basis vectors of the enlarged cell, are

x, y, z	$x, \bar{y}, \bar{z} + 1/2$	$\bar{x}, y, \bar{z}$
x, y, z	$x, \bar{y}, \bar{z}$	$\bar{x}, y, \bar{z} + 1/2.$

(2) **G**: Layer group $pm2_1b$ (L28)

IIb [2] $pm2_1n$ ($\mathbf{a}' = 2\mathbf{a}$)

This entry represents two subgroups whose generators, apart from the translations of the enlarged cell, are

$x, y, z \quad \bar{x}+1/2, y, z \quad \bar{x}, y+1/2, \bar{z}$
$x, y, z \quad \bar{x}, y, z \quad \bar{x}+1/2, y+1/2, \bar{z}.$

The difference between the two subgroups represented by the one entry is due to the different sets of symmetry operations of **G** which are retained in **S**. This can also be expressed as different conventional origins of **S** with respect to **G**: the two subgroups in the first example above are related by a translation **c**/4 of the origin, and the two subgroups in the second example by **a**/4.

1.2.15.2. Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

Another set of *klassengleiche* subgroups is that listed under **IIc**, *i.e.* the subgroups **S** which are of the same or of the enantiomorphic subperiodic group type as **G**. Again, one entry may correspond to more than one isotypic subgroup:

(*a*) As in block **IIb**, one entry may correspond to two isotypic subgroups whose difference can be expressed as different conventional origins of **S** with respect to **G**.

(*b*) One entry may correspond to two isotypic subgroups of equal index but with cell enlargements in different directions which are conjugate subgroups in the affine normalizer of **G**. The different vector relationships are given, separated by 'or' and placed within one pair of parentheses; *cf.* example (2).

Examples

(1) **G**: Rod group $\not{p}222$ (R13)
IIc [2] $\not{p}222$ ($\mathbf{c}' = 2\mathbf{c}$)

This entry corresponds to two isotypic subgroups. Apart from the translations of the enlarged cell, the generators of the subgroups are

$x, y, z \quad x, \bar{y}, \bar{z} \quad \bar{x}, y, \bar{z}$
$x, y, z \quad x, \bar{y}, \bar{z}+1/2 \quad \bar{x}, y, \bar{z}+1/2$

(2) **G**: Layer group *pmm*2 (L23)
IIc [2] *pmm*2 ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$)

This entry corresponds to four isotypic subgroups, two with the enlarged cell with $\mathbf{a}' = 2\mathbf{a}$ and two with the enlarged cell with $\mathbf{b}' = 2\mathbf{b}$. The generators of these subgroups are

$\mathbf{a}' = 2\mathbf{a} \quad \mathbf{b}' = \mathbf{b} \quad x, y, z \quad \bar{x}, y, z \quad x, \bar{y}, z$
$\mathbf{a}' = 2\mathbf{a} \quad \mathbf{b}' = \mathbf{b} \quad x, y, z \quad \bar{x}+1/2, y, z \quad x, \bar{y}, z$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = 2\mathbf{b} \quad x, y, z \quad \bar{x}, y, z \quad x, \bar{y}, z$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = 2\mathbf{b} \quad x, y, z \quad \bar{x}, y+1/2, z \quad x, \bar{y}, z$

(3) **G**: Rod group $\not{p}4_1$ (R24)
IIc [3] $\not{p}4_3$ ($\mathbf{c}' = 3\mathbf{c}$)
[5] $\not{p}4_1$ ($\mathbf{c}' = 5\mathbf{c}$)

Listed here are both the maximal isotypic subgroup $\not{p}4_1$ and the maximal enantiomorphic subgroup $\not{p}4_3$, each of lowest index.

1.2.15.3. Minimal non-isotypic non-enantiomorphic supergroups

If **G** is a maximal subgroup of a group **H**, then **H** is called a minimal supergroup of **G**. Minimal supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the *t* supergroups **I** of **G**, the listing contains the index [*i*] of **G** in **H** and the *conventional* Hermann–Mauguin symbol of **H**. For the *k* supergroups **II**, the subdivision between **IIa** and **IIb** is not made. The information given is similar to that for the subgroups **IIb**, *i.e.* the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of **H**. Note that either the conventional cell of the *k* supergroup **H** is smaller than that of the subperiodic group **G**, or **H** contains additional centring translations.

*Example: **G**: Layer group $p2_1/m11$ (L15)*

Minimal non-isotypic non-enantiomorphic supergroups:

I [2] *pmam*; [2] *pmma*; [2] *pbma*; [2] *pmmn*
II [2] $c2/m11$; [2] $p2/m11$ ($2\mathbf{a}' = \mathbf{a}$)

Block **I** lists [2] *pmam*, [2] *pmma* and [2] *pmmn*. Looking up the *subgroup* data of these three groups one finds [2] $p2_1/m11$. Block **I** also lists [2] *pbma*. Looking up the *subgroup* data of this group one finds [2] $p12_1/m1$ ($p2_1/m11$). This shows that the setting of *pbma* does not correspond to that of $p2_1/m11$ but rather to $p12_1/m1$. To obtain the supergroup **H** referred to the basis of $p2_1/m11$, the basis vectors **a** and **b** must be interchanged. This changes *pbma* to *pmba*, which is the correct symbol of the supergroup of $p2_1/m11$.

Block **II** contains two entries: the first where the conventional cells are the same with the supergroup having additional centring translations, and the second where the conventional cell of the supergroup is smaller than that of the original subperiodic group.

1.2.15.4. Minimal isotypic supergroups and enantiomorphic supergroups of lowest index

No data are listed for *supergroups* **IIc**, because they can be derived directly from the corresponding data of *subgroups* **IIc**.

*Example: **G**: Rod group $\not{p}4_2/m$ (R29)*

The maximal isotypic subgroup of lowest index of $\not{p}4_2/m$ is found in block **IIc**: [3] $\not{p}4_2/m$ ($\mathbf{c}' = 3\mathbf{c}$). By interchanging $\mathbf{c}'$ and **c**, one obtains the minimal isotypic supergroup of lowest index, *i.e.* [3] $\not{p}4_2/m$ ($3\mathbf{c}' = \mathbf{c}$).

1.2.16. Nomenclature

There exists a wide variety of nomenclature for layer, rod and frieze groups (Holser, 1961). Layer-group nomenclature includes *zweidimensionale Raumgruppen* (Alexander & Herrmann, 1929*a*,*b*), *Ebenengruppen* (Weber, 1929), *Netzgruppen* (Hermann, 1929*a*), *net groups* (*IT*, 1952; Opechowski, 1986), *reversal space groups in two dimensions* (Cochran, 1952), *plane groups in three dimensions* (Dornberger-Schiff, 1956, 1959; Belov, 1959), *black and white space groups in two dimensions* (Mackay, 1957), (*two-sided*) *plane groups* (Holser, 1958), *Schichtgruppen* (Niggli, 1959; Chapuis, 1966), *diperiodic groups in three dimensions* (Wood, 1964*a*,*b*), *layer space groups* (Shubnikov & Koptsik, 1974), *layer groups* (Köhler, 1977; Koch & Fischer, 1978; Vainshtein, 1981; Goodman, 1984; Litvin, 1989), *two-dimensional* (*subperiodic*) *groups in three-dimensional space* (Brown *et al.*, 1978) and *plane space groups in three dimensions* (Grell *et al.*, 1989).

Rod-group nomenclature includes *Kettengruppen* (Hermann, 1929*a*,*b*), *eindimensionalen Raumgruppen* (Alexander, 1929, 1934), (*crystallographic*) *line groups in three dimensions* (*IT*, 1952; Opechowski, 1986), *rod groups* (Belov, 1956; Vujicic *et al.*, 1977; Köhler, 1977; Koch & Fischer, 1978), *Balkengruppen*

Table 1.2.17.1. *Frieze-group symbols*

	1	2	3	4	5	6	7	8	9	10	11
Oblique	1	$\not r1$	$r1$	$r1$	$r111$	(a)	t	1	$p[1](1)1$	$r1$	$\not r1$
	2	$\not r211$	$r\bar{1}'$	$r112$	$r112$	$(a) : 2$	$t : 2$	5	$p[2](1)1$	$r2$	$\not r112$
Rectangular	3	$\not r1m1$	$r\bar{1}$	$r1m$	$rm11$	$(a) : m$	$t : m$	3	$p[1](1)m$	$r1m$	$\not rm11$
	4	$\not r11m$	$r11'$	rm	$r1m1$	$(a) \cdot m$	$t \cdot m$	2	$p[1](m)1$	$r11m$	$\not r1m1$
	5	$\not r11g$	$r_2 1$	rg	$r1c1$	$(a) \cdot \bar{a}$	$t \cdot a$	4	$p[1](c)1$	$r11g$	$\not r1a1$
	6	$\not r2mm$	$r\bar{1}1'$	$rmm2$	$rmm2$	$(a) : 2 \cdot m$	$t : 2 \cdot m$	6	$p[2](m)m$	$r2mm$	$\not rmm2$
	7	$\not r2mg$	$r_2\bar{1}$	$rgm2$	$rmc2$	$(a) : 2 \cdot \bar{a}$	$t : 2 \cdot a$	7	$p[2](c)m$	$r2mg$	$\not rma2$

(Niggli, 1959; Chapuis, 1966), *stem groups* (Galyarskii & Zamorzaev, 1965*a*,*b*), *linear space groups* (Bohm & Dornberger-Schiff, 1966) and *one-dimensional* (*subperiodic*) *groups in three dimensions* (Brown *et al.*, 1978).

Frieze-group nomenclature includes *Bortenornamente* (Speiser, 1927), *Bandgruppen* (Niggli, 1959), *line groups* (*borders*) *in two dimensions* (*IT*, 1952), *line groups in a plane* (Belov, 1956), *eindimensionale 'zweifarbige' Gruppen* (Nowacki, 1960), groups of *one-sided bands* (Shubnikov & Koptsik, 1974), *ribbon groups* (Köhler, 1977), *one-dimensional* (*subperiodic*) *groups in two-dimensional space* (Brown *et al.*, 1978) and *groups of borders* (Vainshtein, 1981).

1.2.17. Symbols

The following general criterion was used in selecting the sets of symbols for the subperiodic groups: *consistency with the symbols used for the space groups given in IT* A (2005). Specific criteria following from this general criterion are as follows:

(1) The symbols of subperiodic groups are to be of the Hermann–Mauguin (international) type. This is the type of symbol used for space groups in *IT* A (2005).

(2) A symbol of a subperiodic group is to consist of a letter indicating the lattice centring type followed by a set of characters indicating symmetry elements. This is the format of the Hermann–Mauguin (international) space-group symbols in *IT* A (2005).

(3) The sets of symmetry directions and their sequences in the symbols of the subperiodic groups are those of the corresponding space groups. Layer and rod groups are three-dimensional subperiodic groups of the three-dimensional space groups, and frieze groups are two-dimensional subperiodic groups of the two-dimensional space groups. Consequently, the symmetry directions and sequence of the characters indicating symmetry elements in layer and rod groups are those of the three-dimensional space groups; in frieze groups, they are those of the two-dimensional space groups, see Table 1.2.4.1 above and Table 2.2.4.1 of *IT* A (2005). Layer groups appear as subgroups of three-dimensional space groups, as factor groups of three-dimensional reducible space groups (Kopský, 1986, 1988, 1989*a*,*b*, 1993; Fuksa & Kopský, 1993) and as the symmetries of planes which transect a crystal of a given three-dimensional space-group symmetry. For example, the layer group *pmm*2 is a subgroup of the three-dimensional space group *Pmm*2; is isomorphic to the factor group $Pmm2/T_z$ of the three-dimensional space group *Pmm*2, where T_z is the translational subgroup of all translations along the z axis; and is the symmetry of the plane transecting a crystal of three-dimensional space-group symmetry *Pmm*2, perpendicular to the z axis, at $z = 0$. In these examples, the symbols for the three-dimensional space group and the related subperiodic layer group differ only in the letter indicating the lattice type.

A survey of sets of symbols that have been used for the subperiodic groups is given below. Considering these sets of symbols in relation to the above criteria leads to the sets of symbols for subperiodic groups used in Parts 2, 3 and 4.

1.2.17.1. Frieze groups

A list of sets of symbols for the frieze groups is given in Table 1.2.17.1. The information provided in this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 2.

Columns 3, 4 and 5: symbols listed by Opechowski (1986).

Column 6: symbols listed by Shubnikov & Koptsik (1974).

Column 7: symbols listed by Vainshtein (1981).

Columns 8 and 9: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1967).

Column 10: symbols listed by Lockwood & Macmillan (1978).

Column 11: symbols listed by Shubnikov & Koptsik (1974).

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the set of symbols of the 'black and white' symmetry type (column 3) and the sets of symbols in columns 6 and 7. The sets of symbols in columns 4, 5 and 11 do not follow the sequence of symmetry directions used for two-dimensional space groups. The sets of symbols in columns 3, 4, 5 and 10 do not use a lower-case script $\not r$ to denote a one-dimensional lattice. The set of symbols in column 9 uses parentheses and square brackets to denote specific symmetry directions. The symbol *g* is used in Part 1 to denote a glide line, a standard symbol for two-dimensional space groups (*IT* A, 2005). A letter identical with a basis-vector symbol, *e.g.* *a* or *c*, is not used to denote a glide line, as is done in the symbols of columns 5, 6, 7, 9 and 11, as such a letter is a standard notation for a three-dimensional glide plane (*IT* A, 2005).

Columns 2 and 3 show the isomorphism between frieze groups and one-dimensional magnetic space groups. The one-dimensional space groups are denoted by $\not r1$ and $\not r\bar{1}$. The list of symbols in column 3, on replacing r with $\not r$, is the list of one-dimensional magnetic space groups. The isomorphism between these two sets of groups interexchanges the elements $\bar{1}$ and $1'$ of the one-dimensional magnetic space groups and, respectively, the elements m_x and m_y, mirror lines perpendicular to the [10] and [01] directions, of the frieze groups.

1.2.17.2. Rod groups

A list of sets of symbols for the rod groups is given in Table 1.2.17.2. The information provided in the columns of this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 3.

Columns 3 and 4: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1966, 1967).

Columns 5, 6 and 7: sequential numbering and two sets of symbols listed by Shubnikov & Koptsik (1974).

Table 1.2.17.2. *Rod-group symbols*

	1	2	3	4	5	6	7	8	9
Triclinic	1	$\not{1}$	1	$P(11)1$	1	$(a)\cdot 1$	$p1$	$r1$	$1P1$
	2	$\not{1}\bar{1}$	2	$P(\bar{1}\bar{1})\bar{1}$	7	$(a)\cdot\bar{1}$	$p\bar{1}$	$r\bar{1}$	$1P\bar{1}$
Monoclinic/inclined	3	$\not{2}11$	6	$P(12)1$	2	$(a):2$	$p112$	$r112$	$1P2$
	4	$\not{m}11$	3	$P(1m)1$	22	$(a)\cdot m$	$p11m$	$r1m1$	$mP1$
	5	$\not{c}11$	5	$P(1c)1$	24	$(a)\cdot\bar{a}$	$p11a$	$r1c1$	$gP1$
	6	$\not{2}/m11$	9	$P(12/m)1$	25	$(a):2:m$	$p112/m$	$r12/m1$	$mP2$
	7	$\not{2}/c11$	12	$P(12/c)1$	28	$(a):2:\bar{a}$	$p112/a$	$r12/c1$	$gP2$
Monoclinic/orthogonal	8	$\not{1}12$	7	$P(11)2$	3	$(a)\cdot 2$	$p211$	$r211$	$2P1$
	9	$\not{1}12_1$	8	$P(11)2_1$	8	$(a)\cdot 2_1$	$p2_1$	$r2_1$	2_1P1
	10	$\not{1}1m$	4	$P(11)m$	23	$(a):m$	$pm11$	$rm11$	$1Pm$
	11	$\not{1}12/m$	10	$P(11)2/m$	26	$(a)\cdot 2:m$	$p2/m11$	$r2/m11$	$2Pm$
	12	$\not{1}12_1/m$	11	$P(11)2_1/m$	27	$(a)\cdot 2_1:m$	$p2_1/m11$	$r2_1/m11$	2_1Pm
Orthorhombic	13	$\not{2}22$	18	$P(22)2$	61	$(a)\cdot 2:2$	$p222$	$r222$	$2P22$
	14	$\not{2}22_1$	19	$P(22)2_1$	62	$(a)\cdot 2_1:2$	$p2_122$	$r2_122$	2_1P22
	15	$\not{m}m2$	13	$P(mm)2$	34	$(a)\cdot 2\cdot m$	$p2mm$	$r2mm$	$2mmP1$
	16	$\not{c}c2$	16	$P(cc)2$	35	$(a)\cdot 2\cdot\bar{a}$	$p2aa$	$r2cc$	$2ggP1$
	17	$\not{m}c2_1$	15	$P(mc)2_1$	36	$(a)\cdot 2_1\cdot m$	$p2_1ma$	$r2_1mc$	2_1mgP1
	18	$\not{2}mm$	14	$P(2m)m$	33	$(a):2\cdot m$	$pmma$	$rmm2$	$mPm2$
	19	$\not{2}cm$	17	$P(2c)m$	37	$(a):2\cdot\bar{a}$	$pma2$	$rmc2$	$gPm2$
	20	$\not{m}mm$	20	$P(2/m2/m)2/m$	46	$(a)\cdot m\cdot 2:m$	$pmmm$	$r2/m2/m2/m$	$mmPm$
	21	$\not{c}cm$	21	$P(2/c2/c)2/m$	47	$(a)\cdot\bar{a}\cdot 2:m$	$pmaa$	$r2/m2/c2/c$	$ggPm$
	22	$\not{m}cm$	22	$P(2/m2/c)2_1/m$	48	$(a)\cdot m\cdot 2_1:m$	$pmma$	$r2_1/m2/m2/c$	$mgPm$
Tetragonal	23	$\not{4}$	26	$P4(11)$	5	$(a)\cdot 4$	$p4$	$r4$	$4P1$
	24	$\not{4}_1$	27	$P4_1(11)$	11	$(a)\cdot 4_1$	$p4_1$	$r4_1$	4_1P1
	25	$\not{4}_2$	28	$P4_2(11)$	12	$(a)\cdot 4_2$	$p4_2$	$r4_2$	4_2P1
	26	$\not{4}_3$	29	$P4_3(11)$	13	$(a)\cdot 4_3$	$p4_3$	$r4_3$	4_3P1
	27	$\not{4}\bar{4}$	23	$P\bar{4}(11)$	20	$(a)\cdot\bar{4}$	$p\bar{4}$	$r\bar{4}$	$1P\bar{4}$
	28	$\not{4}/m$	30	$P4/m(11)$	29	$(a)\cdot 4:m$	$p4/m$	$r4/m$	$4Pm$
	29	$\not{4}_2/m$	31	$P4_2/m(11)$	30	$(a)\cdot 4_2:m$	$p4_2/m$	$r4_2/m$	4_2Pm
	30	$\not{4}22$	35	$P4(22)$	66	$(a)\cdot 4:2$	$p422$	$r422$	$4P22$
	31	$\not{4}_122$	36	$P4_1(22)$	67	$(a)\cdot 4_1:2$	$p4_122$	$r4_122$	4_1P22
	32	$\not{4}_222$	37	$P4_2(22)$	68	$(a)\cdot 4_2:2$	$p4_222$	$r4_222$	4_2P22
	33	$\not{4}_322$	38	$P4_3(22)$	69	$(a)\cdot 4_3:2$	$p4_322$	$r4_322$	4_3P22
	34	$\not{4}mm$	32	$P4(mm)$	40	$(a)\cdot 4\cdot m$	$p4mm$	$r4mm$	$4mmP1$
	35	$\not{4}_2cm$	33	$P4_2(cm)$	42	$(a)\cdot 4_2\cdot m$	$p4_2ma$	$r4_2mc$	4_2mgP1
	36	$\not{4}cc$	34	$P4(cc)$	41	$(a)\cdot 4\cdot\bar{a}$	$p4aa$	$r4cc$	$4ggP1$
	37	$\not{4}\bar{4}2m$	24	$P\bar{4}(2m)$	49	$(a)\cdot\bar{4}\cdot m$	$p\bar{4}2m$	$r\bar{4}m2$	$mP\bar{4}2$
	38	$\not{4}\bar{4}2c$	25	$P\bar{4}(2c)$	50	$(a)\cdot\bar{4}\cdot\bar{a}$	$p\bar{4}2a$	$r\bar{4}c2$	$gP\bar{4}2$
	39	$\not{4}/mmm$	39	$P4/m(2/m2/m)$	53	$(a)\cdot m\cdot 4:m$	$p4/mmm$	$r4/m2/m2/m$	$4mmPm$
	40	$\not{4}/mmc$	40	$P4/m(2/c2/c)$	54	$(a)\cdot\bar{a}\cdot 4:m$	$p4/maa$	$r4/m2/c2/c$	$4ggPm$
	41	$\not{4}_2/mmc$	41	$P4_2/m(2/m2/c)$	55	$(a)\cdot m\cdot 4_2:m$	$p4_2/mma$	$r4_2/m2/m2/c$	4_2mgPm
Trigonal	42	$\not{3}$	42	$P3(11)$	4	$(a)\cdot 3$	$p3$	$r3$	$3P1$
	43	$\not{3}_1$	43	$P3_1(11)$	9	$(a)\cdot 3_1$	$p3_1$	$r3_1$	3_1P1
	44	$\not{3}_2$	44	$P3_2(11)$	10	$(a)\cdot 3_2$	$p3_2$	$r3_2$	3_2P1
	45	$\not{3}\bar{3}$	45	$P\bar{3}(11)$	19	$(a)\cdot\bar{6}$	$p\bar{3}$	$r\bar{3}$	$3P\bar{1}$
	46	$\not{3}12$	48	$P3(21)$	63	$(a)\cdot 3:2$	$p32$	$r32$	$3P2$
	47	$\not{3}_112$	49	$P3_1(21)$	64	$(a)\cdot 3_1:2$	$p3_12$	$r3_12$	3_1P2
	48	$\not{3}_212$	50	$P3_2(21)$	65	$(a)\cdot 3_2:2$	$p3_22$	$r3_22$	3_2P2
	49	$\not{3}m1$	46	$P3(m1)$	38	$(a)\cdot 3\cdot m$	$p3m$	$r3m$	$3mP1$
	50	$\not{3}c1$	47	$P3(c1)$	39	$(a)\cdot 3\cdot\bar{a}$	$p3a$	$r3c$	$3gP1$
	51	$\not{3}\bar{3}1m$	51	$P\bar{3}(m1)$	59	$(a)\cdot\bar{6}\cdot m$	$p\bar{3}m$	$r\bar{3}2/m$	$3mP\bar{1}2$
	52	$\not{3}\bar{3}1c$	52	$P\bar{3}(c1)$	60	$(a)\cdot\bar{6}\cdot\bar{a}$	$p\bar{3}a$	$r\bar{3}2/c$	$3gP\bar{1}2$
Hexagonal	53	$\not{6}$	56	$P6(11)$	6	$(a)\cdot 6$	$p6$	$r6$	$6P1$
	54	$\not{6}_1$	57	$P6_1(11)$	14	$(a)\cdot 6_1$	$p6_1$	$r6_1$	6_1P1
	55	$\not{6}_2$	59	$P6_2(11)$	15	$(a)\cdot 6_2$	$p6_2$	$r6_2$	6_2P1
	56	$\not{6}_3$	61	$P6_3(11)$	16	$(a)\cdot 6_3$	$p6_3$	$r6_3$	6_3P1
	57	$\not{6}_4$	60	$P6_4(11)$	17	$(a)\cdot 6_4$	$p6_4$	$r6_4$	6_4P1
	58	$\not{6}_5$	58	$P6_5(11)$	18	$(a)\cdot 6_5$	$p6_5$	$r6_5$	6_5P1
	59	$\not{6}\bar{6}$	53	$P\bar{6}(11)$	21	$(a)\cdot 3:m$	$p\bar{6}$	$r\bar{6}$	$3Pm$
	60	$\not{6}/m$	62	$P6/m(11)$	31	$(a)\cdot 6:m$	$p6/m$	$r6/m$	$6Pm$
	61	$\not{6}_3/m$	63	$P6_3/m(11)$	32	$(a)\cdot 6_3:m$	$p6_3/m$	$r6_3/m$	6_3Pm
	62	$\not{6}22$	67	$P6(22)$	70	$(a)\cdot 6:2$	$p622$	$r622$	$6P22$
	63	$\not{6}_122$	68	$P6_1(22)$	71	$(a)\cdot 6_1:2$	$p6_122$	$r6_122$	6_1P22
	64	$\not{6}_222$	70	$P6_2(22)$	72	$(a)\cdot 6_2:2$	$p6_222$	$r6_222$	6_2P22

Table 1.2.17.2 (*cont.*)

	1	2	3	4	5	6	7	8	9
	65	$\not{6}_3 22$	72	$P6_3(22)$	73	$(a)\cdot 6_3 : 2$	$p6_3 22$	$r6_3 22$	$6_3 P22$
	66	$\not{6}_4 22$	71	$P6_4(22)$	74	$(a)\cdot 6_4 : 2$	$p6_4 22$	$r6_4 22$	$6_4 P22$
	67	$\not{6}_5 22$	69	$P6_5(22)$	75	$(a)\cdot 6_5 : 2$	$p6_5 22$	$r6_5 22$	$6_5 P22$
	68	$\not{6}mm$	64	$P6(mm)$	43	$(a)\cdot 6\cdot m$	$p6mm$	$r6mm$	$6mmP1$
	69	$\not{6}cc$	65	$P6(cc)$	44	$(a)\cdot 6\cdot \bar{a}$	$p6aa$	$r6cc$	$6ggP1$
	70	$\not{6}_3 mc$	66	$P6_3(cm)$	45	$(a)\cdot 6_3\cdot m$	$p6_3 ma$	$r6_3 mc$	$6_3 mgP1$
	71	$\not{6}\bar{6}m2$	54	$P\bar{6}(m2)$	51	$(a)\cdot m\cdot 3 : m$	$p\bar{6}m2$	$r\bar{6}m2$	$3mPm2$
	72	$\not{6}\bar{6}c2$	55	$P\bar{6}(c2)$	52	$(a)\cdot \bar{a}\cdot 3 : m$	$p\bar{6}a2$	$r\bar{6}c2$	$3gPm2$
	73	$\not{6}/mmm$	73	$P6/m(2/m2/m)$	56	$(a)\cdot m\cdot 6 : m$	$p6/mmm$	$r6/m2/m2/m$	$6mmPm$
	74	$\not{6}/mcc$	74	$P6/m(2/c2/c)$	57	$(a)\cdot \bar{a}\cdot 6 : m$	$p6/maa$	$r6/m2/c2/c$	$6ggPm$
	75	$\not{6}_3/mmc$	75	$P6_3/m(2/c2/m)$	58	$(a)\cdot m\cdot 6_3 : m$	$p6_3/mma$	$r6_3/m2/m2/c$	$6_3 mgPm$

Column 8: symbols listed by Opechowski (1986).

Column 9: symbols listed by Niggli (Chapuis, 1966).

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the set of symbols in column 6 and the Niggli-type set of symbols in column 9. The set of symbols in column 8 does not use the lower-case script letter $\not{}$, as does *IT* A (2005), to denote a one-dimensional lattice. The order of the characters indicating symmetry elements in the set of symbols in column 7 does not follow the sequence of symmetry directions used for three-dimensional space groups. The set of symbols in column 4 have the characters indicating symmetry elements along non-lattice directions enclosed in parentheses, and do not use a lower-case script letter to denote the one-dimensional lattice. Lastly, the set of symbols in column 4, without the parentheses and with the one-dimensional lattice denoted by a lower-case script $\not{}$, are identical with the symbols in Part 3, or in some cases are the second setting of rod groups whose symbols are given in Part 3. These second-setting symbols are included in the symmetry diagrams of the rod groups.

1.2.17.3. Layer groups

A list of sets of symbols for the layer groups is given in Table 1.2.17.3. The information provided in the columns of this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 4.

Columns 3 and 4: sequential numbering and symbols listed by Wood (1964*a*,*b*) and Litvin & Wike (1991).

Columns 5 and 6: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1966, 1967).

Columns 7 and 8: sequential numbering and symbols listed by Shubnikov & Koptsik (1974) and Vainshtein (1981).

Column 9: symbols listed by Holser (1958).

Column 10: sequential numbering listed by Weber (1929).

Column 11: symbols listed by Hermann (1929*a*,*b*).

Column 12: symbols listed by Alexander & Herrmann (1929*a*,*b*).

Column 13: symbols listed by Niggli (Wood, 1964*a*,*b*).

Column 14: symbols listed by Shubnikov & Koptsik (1974).

Columns 15 and 16: symbols listed by Aroyo & Wondratschek (1987).

Column 17: symbols listed by Belov *et al.* (1957*a*,*b*).

Columns 18 and 19: symbols and sequential numbering listed by Belov & Tarkhova (1956*a*,*b*,*c*,*d*).

Columns 20 and 21: symbols listed by Cochran as listed, respectively, by Cochran (1952) and Belov & Tarkhova (1956*a*,*b*,*c*,*d*).

Column 22: symbols listed by Opechowski (1986).

Column 23: symbols listed by Grunbaum & Shephard (1987).

Column 24: symbols listed by Woods (1935*a*,*b*,*c*, 1936).

Column 25: symbols listed by Coxeter (1986).

There is also a notation for layer groups, introduced by Janovec (1981), in which all elements in the group symbol which change the direction of the normal to the plane containing the translations are underlined, *e.g.* $p4/\underline{m}$. However, we know of no listing of all layer-group types in this notation.

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the sets of symbols of the Schoenflies type (columns 11 and 12) and symbols of the 'black and white' symmetry type (columns 16, 17, 18, 20, 21, 22, 24 and 25). Additional non-Hermann–Mauguin (international) type sets of symbols are those in columns 14 and 23.

Sets of symbols which do not begin with a letter indicating the lattice centring type are the sets of symbols of the Niggli type (columns 13 and 15). The order of the characters indicating symmetry elements in the sets of symbols in columns 4 and 9 does not follow the sequence of symmetry directions used for three-dimensional space groups. The set of symbols in column 6 uses parentheses to denote a symmetry direction which is not a lattice direction. In addition, the set of symbols in column 6 uses upper-case letters to denote the two-dimensional lattice of the layer group, where as in *IT* A (2005) upper-case letters denote three-dimensional lattices.

The symbols in column 8 are either identical with or, in some monoclinic and orthorhombic cases, are the second-setting or alternative-cell-choice symbols of the layer groups whose symbols are given in Part 4. These second-setting and alternative-cell-choice symbols are included in the symmetry diagrams of the layer groups.

The isomorphism between layer groups and two-dimensional magnetic space groups can be seen in Table 1.2.17.3. The set of symbols which we use for layer groups is given in column 2. The sets of symbols in columns 16, 17 and 22 are sets of symbols for the two-dimensional magnetic space groups. The basic relationship between these two sets of groups is the interexchanging of the magnetic symmetry element $1'$ and the layer symmetry element m_z. A detailed discussion of the relationship between these two sets of groups has been given by Opechowski (1986).

References

Alexander, E. (1929). *Systematik der eindimensionalen Raumgruppen. Z. Kristallogr.* **70**, 367–382.

Alexander, E. (1934). *Bemerkung zur Systematik der eindimensionalen Raumgruppen. Z. Kristallogr.* **89**, 606–607.

Table 1.2.17.3. *Layer-group symbols*

(*a*) Columns 1–9.

	1	2	3	4	5	6	7	8	9
Triclinic/oblique	1	$p1$	1	$P1$	1	$P11(1)$	1	$p1$	$p1$
	2	$p\bar{1}$	2	$P\bar{1}$	2	$P\bar{1}\bar{1}(\bar{1})$	3	$p\bar{1}$	$p\bar{1}$
Monoclinic/oblique	3	$p112$	3	$P211$	9	$P11(2)$	5	$p112$	$p21$
	4	$p11m$	4	$Pm11$	4	$P11(m)$	2	$p11m$	$pm1$
	5	$p11a$	5	$Pb11$	5	$P11(b)$	4	$p11b$	$pa1$
	6	$p112/m$	6	$P2/m11$	13	$P11(2/m)$	6	$p112/m$	$p2/m1$
	7	$p112/a$	7	$P2/b11$	17	$P11(2/b)$	7	$p112/b$	$p2/a1$
Monoclinic/rectangular	8	$p211$	8	$P112$	8	$P12(1)$	14	$p121$	$p12$
	9	$p2_111$	9	$P112_1$	10	$P12_1(1)$	15	$p12_11$	$p12_1$
	10	$c211$	10	$C112$	11	$C12(1)$	16	$c121$	$c12$
	11	$pm11$	11	$P11m$	3	$P1m(1)$	8	$p1m1$	$p1m$
	12	$pb11$	12	$P11a$	5	$P1a(1)$	10	$p1a1$	$p1b$
	13	$cm11$	13	$C11m$	7	$C1m(1)$	12	$c1m1$	$c1m$
	14	$p2/m11$	14	$P112/m$	12	$P12/m(1)$	17	$p12/m1$	$p12/m$
	15	$p2_1/m11$	15	$P112_1/m$	14	$P12_1/m(1)$	18	$p12_1/m1$	$p12_1/m$
	16	$p2/b11$	17	$P112/a$	16	$P12/a(1)$	20	$p12/a1$	$p12/b$
	17	$p2_1/b11$	18	$P112_1/a$	18	$P12_1/a(1)$	21	$p12_1/a1$	$p12_1/b$
	18	$c2/m11$	16	$C112/m$	15	$C12/m(1)$	19	$c12/m1$	$c12/m$
Orthorhombic/rectangular	19	$p222$	19	$P222$	33	$P22(2)$	37	$p222$	$p222$
	20	$p2_122$	20	$P222_1$	34	$P2_12(2)$	38	$p2_122$	$p222_1$
	21	$p2_12_12$	21	$P22_12_1$	35	$P2_12_1(2)$	39	$p2_12_12$	$p22_12_1$
	22	$c222$	22	$C222$	36	$C22(2)$	40	$c222$	$c222$
	23	$pmm2$	23	$P2mm$	19	$Pmm(2)$	22	$pmm2$	$p2mm$
	24	$pma2$	28	$P2ma$	24	$Pma(2)$	24	$pbm2$	$p2ma$
	25	$pba2$	33	$P2ba$	29	$Pba(2)$	26	$pba2$	$p2ba$
	26	$cmm2$	34	$C2mm$	30	$Cmm(2)$	28	$cmm2$	$c2mm$
	27	$pm2m$	24	$Pmm2$	20	$P2m(m)$	9	$p2mm$	$pm2m$
	28	$pm2_1b$	26	$Pbm2_1$	21	$P2_1m(a)$	30	$p2_1ma$	$pa2_1m$
	29	$pb2_1m$	25	$Pm2_1a$	22	$P2_1a(m)$	11	$p2_1am$	$pm2_1a$
	30	$pb2b$	27	$Pbb2$	23	$P2a(a)$	31	$p2aa$	$pa2a$
	31	$pm2a$	29	$Pam2$	25	$P2m(b)$	32	$p2mb$	$pb2m$
	32	$pm2_1n$	32	$Pnm2_1$	28	$P2_1m(n)$	35	$p2_1mn$	$pn2_1m$
	33	$pb2_1a$	30	$Pab2_1$	26	$P2_1a(b)$	33	$p2_1ab$	$pb2_1a$
	34	$pb2n$	31	$Pnb2$	27	$P2a(n)$	34	$p2an$	$pn2a$
	35	$cm2m$	35	$Cmm2$	31	$C2m(m)$	13	$c2mm$	$cm2m$
	36	$cm2e$	36	$Cam2$	32	$Cm2(a)$	36	$c2mb$	$cb2m$
	37	$pmmm$	37	$P2/m2/m2/m$	37	$P2/m2/m(2/m)$	23	$pmmm$	$p2/m2/m2/m$
	38	$pmaa$	38	$P2/a2/m2/a$	38	$P2/m2/a(2/a)$	41	$pmaa$	$p2/a2/m2/a$
	39	$pban$	39	$P2/n2/b2/a$	39	$P2/b2/a(2/n)$	42	$pban$	$p2/n2/b2/a$
	40	$pmam$	40	$P2/m2_1/m2/a$	41	$P2/b2_1/m(2/m)$	25	$pbmm$	$p2/m2_1/m2/a$
	41	$pmma$	41	$P2/a2_1/m2/m$	40	$P2_1/m2/m(2/a)$	43	$pmma$	$p2/a2_1/m2/m$
	42	$pman$	42	$P2/n2/m2_1/a$	42	$P2_1/b2/m(2/n)$	44	$pbmn$	$p2/n2/m2_1/a$
	43	$pbaa$	43	$P2/a2/b2_1/a$	43	$P2/b2_1/a(2/a)$	45	$pbaa$	$p2/a2/b2_1/a$
	44	$pbam$	44	$P2/m2_1/b2_1/a$	44	$P2_1/b2_1/a(2/m)$	27	$pbam$	$p2/m2_1/b2_1/a$
	45	$pbma$	45	$P2/a2_1/b2_1/m$	45	$P2_1/m2_1/a(2/b)$	46	$pmab$	$p2/a2_1/b2_1/m$
	46	$pmmn$	46	$P2/n2_1/m2_1/m$	46	$P2_1/m2_1/m(2/n)$	47	$pmmn$	$p2/n2_1/m2_1/m$
	47	$cmmm$	47	$C2/m2/m2/m$	47	$C2/m2/m(2/m)$	29	$cmmm$	$c2/m2/m2/m$
	48	$cmme$	48	$C2/a2/m2/m$	48	$C2/m2/m(2/a)$	48	$cmma$	$c2/a2/m2/m$
Tetragonal/square	49	$p4$	49	$P4$	54	$P(4)11$	50	$p4$	$p4$
	50	$p\bar{4}$	50	$P\bar{4}$	49	$P(\bar{4})11$	49	$p\bar{4}$	$p\bar{4}$
	51	$p4/m$	51	$P4/m$	55	$P(4/m)11$	51	$p4/m$	$p4/m$
	52	$p4/n$	52	$P4/n$	56	$P(4/n)11$	57	$p4/n$	$p4/n$
	53	$p422$	53	$P422$	59	$P(4)22$	55	$p422$	$p422$
	54	$p42_12$	54	$P42_12$	60	$P(4)2_12$	56	$p42_12$	$p42_12$
	55	$p4mm$	55	$P4mm$	57	$P(4)mm$	52	$p4mm$	$p4mm$
	56	$p4bm$	56	$P4bm$	58	$P(4)bm$	59	$p4bm$	$p4bm$
	57	$p\bar{4}2m$	57	$P\bar{4}2m$	50	$P(\bar{4})2m$	54	$p\bar{4}2m$	$p\bar{4}2m$
	58	$p\bar{4}2_1m$	58	$P\bar{4}2_1m$	51	$P(\bar{4})2_1m$	60	$p\bar{4}2_1m$	$p\bar{4}2_1m$
	59	$p\bar{4}m2$	59	$P\bar{4}m2$	52	$P(\bar{4})m2$	61	$p\bar{4}m2$	$p\bar{4}m2$
	60	$p\bar{4}b2$	60	$P\bar{4}b2$	53	$P(\bar{4})b2$	64	$p\bar{4}b2$	$p\bar{4}b2$
	61	$p4/mmm$	61	$P4/m2/m2/m$	61	$P(4/m)2/m2/m$	53	$p4/mmm$	$p4/m2/m2/m$
	62	$p4/nbm$	62	$P4/n2/b2/m$	62	$P(4/n)2/b2/m$	62	$p4/nbm$	$p4/n2/b2/m$

Table 1.2.17.3 (*cont.*)

	1	2	3	4	5	6	7	8	9
	63	$p4/mbm$	63	$P4/m2_1/b2/m$	63	$P(4/m)2_1/b2/m$	58	$p4/mbm$	$p4/m2_1/b2/m$
	64	$p4/nmm$	64	$P4/n2_1/m2/m$	64	$P(4/n)2_1/m2/m$	63	$p4/nmm$	$p4/n2_1/m2/m$
Trigonal/hexagonal	65	$p3$	65	$P3$	65	$P(3)11$	65	$p3$	$p3$
	66	$p\bar{3}$	66	$P\bar{3}$	66	$P(\bar{3})11$	67	$p\bar{3}$	$p\bar{3}$
	67	$p312$	67	$P312$	70	$P(3)12$	72	$p312$	$p312$
	68	$p321$	68	$P321$	69	$P(3)21$	73	$p321$	$p321$
	69	$p3m1$	69	$P3m1$	67	$P(3)m1$	68	$p3m1$	$p3m1$
	70	$p31m$	70	$P31m$	68	$P(3)1m$	70	$p31m$	$p31m$
	71	$p\bar{3}1m$	71	$P\bar{3}12/m$	72	$P(\bar{3}1m$	74	$p\bar{3}1m$	$p\bar{3}12/m$
	72	$p\bar{3}m1$	72	$P\bar{3}2/m1$	71	$P(\bar{3})m1$	75	$p\bar{3}m1$	$p\bar{3}2/m1$
Hexagonal/hexagonal	73	$p6$	73	$P6$	76	$P(6)11$	76	$p6$	$p6$
	74	$p\bar{6}$	74	$P\bar{6}$	73	$P(\bar{6})11$	66	$p\bar{6}$	$p\bar{6}$
	75	$p6/m$	75	$P6/m$	77	$P(6/m)11$	77	$p6/m$	$p6/m$
	76	$p622$	76	$P622$	79	$P(6)22$	80	$p622$	$p622$
	77	$p6mm$	77	$P6mm$	78	$P(6)mm$	78	$p6mm$	$p6mm$
	78	$p\bar{6}m2$	78	$P\bar{6}m2$	74	$P(\bar{6})m2$	69	$p\bar{6}m2$	$p\bar{6}m2$
	79	$p\bar{6}2m$	79	$P\bar{6}2m$	75	$P(\bar{6})2m$	71	$p\bar{6}2m$	$p\bar{6}2m$
	80	$p6/mmm$	80	$P6/m2/m2/m$	80	$P(6/m)2/m2/m$	79	$p6/mmm$	$p6/m2/m2/m$

(*b*) Columns 10–17.

	1	10	11	12	13	14	15	16	17
Triclinic/oblique	1	1	$C_1\bar{p}$	C_1^1	$1P1$	$(a/b)\cdot 1$	$1p1$	$p1$	$p1$
	2	2	$S_2\bar{p}$	C_i^1	$1P\bar{1}$	$(a/b)\cdot\bar{1}$	$1p\bar{1}$	$p2'$	$p2'$
Monoclinic/oblique	3	8	$C_2\bar{p}$	C_2^1	$1P2$	$(a/b):2$	$1p112$	$p2$	$p2$
	4	3	$C_{1h}\bar{p}\mu$	C_{1h}^1	$mP1$	$(a/b)\cdot m$	$mp1$	p^*1	
	5	4	$C_{1h}\bar{p}\alpha$	C_{1h}^2	$aP1$	$(a/b)\cdot\bar{b}$	$bp1$	$p'_{b'}1$	p'_b1
	6	12	$C_{2h}\bar{p}\mu$	C_{2h}^1	$mP2$	$(a/b)\cdot m:2$	$mp112$	p^*2	
	7	13	$C_{2h}\bar{p}\alpha$	C_{2h}^2	$aP2$	$(a/b)\cdot\bar{b}:2$	$bp112$	$p'_{b'}2$	p'_b2
Monoclinic/rectangular	8	9	$D_1\bar{p}1$	C_2^2	$1P12$	$(a:b)\cdot 2$	$1p12$	$p1m'1$	pm'
	9	10	$D_1\bar{p}2$	C_2^3	$1P12_1$	$(a:b)\cdot 2_1$	$1p12_1$	$p1g'1$	pg'
	10	11	$D_1\bar{c}1$	C_2^4	$1C12$	$\left(\frac{a+b}{2}/a:b\right)\cdot 2$	$1c12$	$c1m'1$	cm'
	11	5	$C_{1v}\bar{p}\mu$	C_{1h}^3	$1P1m$	$(a:b):m$	$1p1m$	$p11m$	pm
	12	6	$C_{1v}\bar{p}\beta$	C_{1h}^4	$1P1g$	$(a:b):\bar{a}$	$1p1a$	$p11g$	pg
	13	7	$C_{1v}\bar{c}\mu$	C_{1h}^5	$1C1m$	$\left(\frac{a+b}{2}/a:b\right):m$	$1c1m$	$c11m$	cm
	14	14	$D_{1d}\bar{p}\mu1$	C_{2h}^3	$1P12/m$	$(a:b)\cdot 2:m$	$1p12/m$	$p2'm'm$	$pm'm$
	15	15	$D_{1d}\bar{p}\mu2$	C_{2h}^5	$1P12_1/m$	$(a:b)\cdot 2_1:m$	$1p12_1/m$	$p2'g'm$	$pg'm$
	16	18	$D_{1d}\bar{p}\beta2$	C_{2h}^6	$1P12/g$	$(a:b)\cdot 2\cdot\bar{a}$	$1p12_1/a$	$p2'g'g$	$pg'g$
	17	17	$D_{1d}\bar{p}\beta1$	C_{2h}^4	$1P12_1/g$	$(a:b)\cdot 2_1:\bar{a}$	$1p12/a$	$p2'm'g$	$pm'g$
	18	16	$D_{1d}\bar{c}\mu1$	C_{2h}^7	$1C12/m$	$\left(\frac{a+b}{2}/a:b\right)\cdot 2:m$	$1c12/m$	$c2'm'm$	$cm'm$
Orthorhombic/rectangular	19	33	$D_2\bar{p}11$	V^1	$1P222$	$(a:b):2:2$	$1p222$	$p2m'm'$	$pm'm'$
	20	34	$D_2\bar{p}12$	V^3	$1P222_1$	$(a:b):2:2_1$	$1p22_12$	$p2g'm'$	$pm'g'$
	21	35	$D_2\bar{p}22$	V^2	$1P22_12_1$	$(a:b)\cdot 2_1:2_1$	$1p2_12_12$	$p2g'g'$	$pg'g'$
	22	36	$D_2\bar{c}11$	V^4	$1C222$	$\left(\frac{a+b}{2}/a:b\right):2:2$	$1c222$	$c2m'm'$	$cm'm'$
	23	19	$C_{2v}\bar{p}\mu\mu$	C_{2v}^1	$1P2mm$	$(a:b):2\cdot m$	$1pmm2$	$p2mm$	pmm
	24	20	$C_{2v}\bar{p}\mu\alpha$	C_{2v}^2	$1P2mg$	$(a:b):2\cdot\bar{b}$	$1pma2$	$p2mg$	pmg
	25	21	$C_{2v}\bar{p}\beta\alpha$	C_{2v}^{10}	$1P2gg$	$(a:b):\bar{a}:\bar{b}$	$1pba2$	$p2gg$	pgg
	26	22	$C_{2v}\bar{c}\mu\mu$	C_{2v}^3	$1C2mm$	$\left(\frac{a+b}{2}/a:b\right):m\cdot 2$	$1cmm2$	$c2mm$	cmm
	27	23	$D_{1h}\bar{p}\mu\mu$	C_{2v}^4	$mP12m$	$(a:b)\cdot m\cdot 2$	$mpm2$	p^*1m1	
	28	25	$D_{1h}\bar{p}\beta\mu$	C_{2v}^5	$aP12_1m$	$(a:b):m\cdot 2_1$	$bpm2_1$	$p'_{b'}1m1$	p'_a1m
	29	24	$D_{1h}\bar{p}\mu\beta$	C_{2v}^7	$mP12_1g$	$(a:b)\cdot m\cdot 2_1$	$mpb2_1$	p^*1g1	
	30	26	$D_{1h}\bar{p}\beta\beta$	C_{2v}^6	$aP12g$	$(a:b)\cdot\bar{a}\cdot 2$	$bpb2$	$p'_{b'}1m'1$	p'_a1g
	31	27	$D_{1h}\bar{p}\alpha\mu$	C_{2v}^{11}	$bP12m$	$(a:b)\cdot\bar{b}\cdot 2$	$apm2$	$p'_{a'}1m1$	p'_b1m
	32	30	$D_{1h}\bar{p}\upsilon\mu$	C_{2v}^{13}	$nP12_1m$	$(a:b)\cdot ab\cdot 2_1$	$npm2_1$	$c'1m1$	p'_c1m
	33	28	$D_{1h}\bar{p}\alpha\beta$	C_{2v}^{14}	$bP12_1g$	$(a:b)\cdot\bar{b}:\bar{a}$	$apb2_1$	$p'_{a'}1g1$	p'_b1g
	34	29	$D_{1h}\bar{p}\upsilon\beta$	C_{2v}^{12}	$nP12g$	$(a:b)\cdot ab\cdot 2$	$npb2$	$c'1m'1$	p'_c1m'
	35	31	$D_{1h}\bar{c}\mu\mu$	C_{2v}^8	$mC12m$	$\left(\frac{a+b}{2}/a:b\right)\cdot m\cdot 2$	$mcm2$	c^*1m1	
	36	32	$D_{1h}\bar{c}\alpha\mu$	C_{2v}^9	$aC12m$	$\left(\frac{a+b}{2}/a:b\right)\cdot\bar{b}\cdot 2$	$acm2$	$p'_{a'b'}1m1$	$c'1m$
	37	37	$D_{2h}\bar{p}\mu\mu\mu$	V_h^1	$mP2mm$	$(a:b)\cdot m:2\cdot m$	$mp2/m2/m2$	p^*2mm	
	38	38	$D_{2h}\bar{p}\alpha\mu\alpha$	V_h^5	$aP2mg$	$(a:b)\cdot\bar{a}:2\cdot\bar{a}$	$ip2/m2/a2$	$p'_{a'}2mg$	p'_amg
	39	39	$D_{2h}\bar{p}\upsilon\beta\alpha$	V_h^6	$nP2gg$	$(a:b)\cdot ab:2\cdot a$	$np2/b2/a2$	$c'2m'm'$	$p'_cm'm'$
	40	40	$D_{2h}\bar{p}\mu\mu\alpha$	V_h^3	$mP2mg$	$(a:b)\cdot m:2\cdot\bar{b}$	$np2_1/m2/a2$	p^*2mg	
	41	41	$D_{2h}\bar{p}\alpha\mu\mu$	V_h^9	$aP2mm$	$(a:b)\cdot\bar{a}:2\cdot m$	$ap2_1/m2/m2$	$p'_{a'}2mm$	p'_bmm
	42	42	$D_{2h}\bar{p}\upsilon\mu\alpha$	V_h^{11}	$nP2mg$	$(a:b)\cdot ab:2\cdot b$	$np2/m2_1/a2$	$c'2mm'$	$p'_cm'm$

Table 1.2.17.3 (*cont.*)

	1	10	11	12	13	14	15	16	17
	43	43	$D_{2h}\bar{p}\alpha\beta\alpha$	V_h^{10}	$aP2gg$	$(a:b)\cdot\bar{a}\cdot 2:\bar{b}$	$ap2/b2_1/a2$	$p'_{a'}2gg$	p'_bgg
	44	44	$D_{2h}\bar{p}\mu\beta\alpha$	V_h^2	$mP2gg$	$(a:b)\cdot m:\bar{a}:\bar{b}$	$np2_1/b2_1/a2$	p^*2gg	
	45	45	$D_{2h}\bar{p}\alpha\beta\mu$	V_h^7	$aP2gm$	$(a:b)\cdot\bar{b}:2\cdot\bar{a}$	$ap2_1/b2_1/m2$	$p'_{a'}2gm$	p'_bmg
	46	46	$D_{2h}\bar{p}\upsilon\mu\mu$	V_h^8	$nP2mm$	$(a:b)\cdot ab:2\cdot m$	$np2_1/m2_1/m2$	$c'2mm$	p'_cmm
	47	47	$D_{2h}\bar{c}\mu\mu\mu$	V_h^4	$mC2mm$	$\left(\frac{a+b}{2}/a:b\right)\cdot m:2\cdot m$	$mc2/m2/m2$	c^*2mm	
	48	48	$D_{2h}\bar{c}\alpha\mu\mu$	V_h^{12}	$aC2mm$	$\left(\frac{a+b}{2}/a:b\right)\cdot\bar{a}:2\cdot m$	$ac2/m2/m2$	$p'_{a'b'}2mm$	$c'mm$
Tetragonal/square	49	58	$C_4\bar{p}$	C_4^1	$1P4$	$(a:a):4$	$1p4$	$p4$	$p4$
	50	57	$S_4\bar{p}$	S_4^1	$1P\bar{4}$	$(a:a):\bar{4}$	$1p\bar{4}$	$p4'$	$p4'$
	51	61	$C_{4h}\bar{p}\mu$	C_{4h}^1	$mP4$	$(a:a):4:m$	$mp4$	p^*4	
	52	62	$C_{4h}\bar{p}\upsilon$	C_{4h}^2	$nP4$	$(a:a):4:ab$	$np4$	$c'4$	$p'4$
	53	67	$D_4\bar{p}11$	D_4^1	$1P422$	$(a:a):4:2$	$1p422$	$p4m'm'$	$p4m'm'$
	54	68	$D_4\bar{p}21$	D_4^2	$1P42_12$	$(a:a):4:2_1$	$1p42_12$	$p4g'm'$	$p4g'm'$
	55	59	$C_{4v}\bar{p}\mu\mu$	C_{4v}^1	$1P4mm$	$(a:a):4\cdot m$	$1p4mm$	$p4mm$	$p4mm$
	56	60	$C_{4v}\bar{p}\beta\mu$	C_{4v}^2	$1P4gm$	$(a:a):4\odot b$	$1p4bm$	$p4gm$	$p4gm$
	57	63	$D_{2d}\bar{p}\mu 1$	V_d^1	$1P\bar{4}2m$	$(a:a):\bar{4}:2$	$1p\bar{4}2m$	$p4'm'm$	$p4'm'm$
	58	64	$D_{2d}\bar{p}\mu 2$	V_d^2	$1P\bar{4}2_1m$	$(a:a):\bar{4}\odot 2_1$	$1p\bar{4}2_1m$	$p4'g'm$	$p4'g'm$
	59	65	$D_{2d}\bar{c}\mu 1$	V_d^3	$1P\bar{4}m2$	$(a:a):\bar{4}\cdot m$	$1p\bar{4}m2$	$p4'mm'$	$p4'mm'$
	60	66	$D_{2d}\bar{c}\beta 1$	V_d^4	$1P\bar{4}g2$	$(a:a):\bar{4}\odot\bar{b}$	$1p\bar{4}b2$	$p4'gm'$	$p4'gm'$
	61	69	$D_{4h}\bar{p}\mu\mu\mu$	D_{4h}^1	$mP4mm$	$(a:a)\cdot m:4\cdot m$	$mp42/m2/m$	p^*4mm	
	62	70	$D_{4h}\bar{p}\upsilon\beta\mu$	D_{4h}^2	$nP4gm$	$(a:a):ab:4\odot b$	$np42/b2/m$	$c'4m'm$	$p'4gm$
	63	71	$D_{4h}\bar{p}\mu\beta\mu$	D_{4h}^3	$mP4gm$	$(a:a)\cdot m:4\odot b$	$mp42_1/b2/m$	p^*4gm	
	64	72	$D_{4h}\bar{p}\upsilon\mu\mu$	D_{4h}^4	$nP4mm$	$(a:a)\cdot ab:4\cdot m$	$np42_1/m2/m$	$c'4mm$	$p'4mm$
Trigonal/hexagonal	65	49	$C_3\bar{c}$	C_3^1	$1P3$	$(a/a):3$	$1p3$	$p3$	$p3$
	66	50	$S_6\bar{p}$	C_{3i}^1	$1P\bar{3}$	$(a/a):\bar{3}$	$1p\bar{3}$	$p6'$	$p6'$
	67	54	$D_3\bar{c}1$	D_3^1	$1P312$	$(a/a):2:3$	$1p312$	$p3m'1$	$p3m'1$
	68	53	$D_3\bar{h}1$	D_3^2	$1P321$	$(a/a)\cdot 2:3$	$1p321$	$p31m'$	$p31m'$
	69	51	$C_{3v}\bar{c}\mu$	C_{3v}^2	$1P3m1$	$(a/a):m\cdot 3$	$1p3m1$	$p3m1$	$p3m1$
	70	52	$C_{3v}\bar{h}\mu$	C_{3v}^1	$1P31m$	$(a/a)\cdot m\cdot 3$	$1p31m$	$p31m$	$p31m$
	71	55	$D_{3d}\bar{c}\mu 1$	D_{3d}^2	$1P\bar{3}1m$	$(a/a)\cdot m\cdot\bar{6}$	$1p\bar{3}12/m$	$p6'm'm$	$p6'm'm$
	72	56	$D_{3d}\bar{h}\mu 1$	D_{3d}^1	$1P\bar{3}m1$	$(a/a):m\cdot\bar{6}$	$1p\bar{3}2/m1$	$p6'mm'$	$p6'mm'$
Hexagonal/hexagonal	73	76	$C_6\bar{c}$	C_6^1	$1P6$	$(a/a):6$	$1p6$	$p6$	$p6$
	74	73	$C_{3h}\bar{c}\mu$	C_{3h}^1	$mP3$	$(a/a):3:m$	$mp3$	p^*3	
	75	78	$C_{6h}\bar{c}\mu$	C_{6h}^1	$mP6$	$(a/a)\cdot m:6$	$mp6$	p^*6	
	76	79	$D_6\bar{c}11$	D_6^1	$1P622$	$(a/a):2:6$	$1p622$	$p6m'm'$	$p6m'm'$
	77	77	$C_{6v}\bar{c}\mu\mu$	C_{6v}^1	$1P6mm$	$(a/a):m\cdot 6$	$1p6mm$	$p6mm$	$p6mm$
	78	74	$D_{3h}\bar{c}\mu\mu$	D_{3h}^1	$mP3m2$	$(a/a):m\cdot 3:m$	$mp3m2$	p^*3m1	
	79	75	$D_{3h}\bar{h}\mu\mu$	D_{3h}^2	$mP32m$	$(a/a)\cdot m:3\cdot m$	$mp32m$	p^*31m	
	80	80	$D_{6h}\bar{c}\mu\mu\mu$	D_{6h}^1	$mP6mm$	$(a/a)\cdot m:6\cdot m$	$mp6mm$	p^*6mm	

(*c*) Columns 18–25.

	1	18	19	20	21	22	23	24	25
Triclinic/oblique	1	$p1$	47			$p1$			
	2	$p2'$	1	$p2'$	$p2^-$	$p2'$	$p2[2]_1$	$2'11$	$p2/p1$
Monoclinic/oblique	3	$p2$	48			$p2$			
	4	$p1'$	64			$p11'$			
	5	p'_b1	2	pt'	pt^-	$p_{2b}1$	$p1[2]$	$b11$	$p1/p1$
	6	$p21'$	65			$p21'$			
	7	p'_b2	3	$p2t'$	$p2t^-$	$p_{2b}2$	$p2[2]_2$	$2/b11$	$p2/p2$
Monoclinic/rectangular	8	pm'	4	pm'	pm^-	pm'	$pm[2]_4$	$12'1$	$pm/p1$
	9	pg'	5	pg'	pg^-	pg'	$pg[2]_1$	$112'_1$	$pg/p1$
	10	cm'	6	cm'	cm^-	cm'	$cm[2]_1$	$c112'$	$cm/p1$
	11	pm	49			pm			
	12	pg	50			pg			
	13	cm	51			cm			
	14	pmm'	14	pmm'	pmm^-	$pm'm$	$pmm[2]_2$	$2'2'2$	pmm/pm
	15	pmg'	17	pmg'	pmg^-	pmg'	$pmg[2]_4$	$2'2'_12$	pmg/pm
	16	pgg'	18	pgg'	pgg^-	pgg'	$pgg[2]_1$	$2'2'_12_1$	pgg/pg
	17	$pm'g$	16	$pm'g$	pm^-g	$pm'g$	$pmg[2]_2$	$2'2_12'$	pmg/pg
	18	cmm'	21	cmm'	cmm^-	cmm'	$cmm[2]_2$	$c2'22'$	cmm/cm
Orthorhombic/rectangular	19	$pm'm'$	15	$pm'm'$	pm^-m^-	$pm'm'$	$pmm[2]_5$	$22'2'$	$pmm/p2$
	20	$pm'g'$	20	$pm'g'$	pm^-g^-	$pm'g'$	$pmg[2]_5$	$22'2'_1$	$pmg/p2$
	21	$pg'g'$	19	$pg'g'$	pg^-g^-	$pg'g'$	$pgg[2]_2$	$22'_12'_1$	$pgg/p2$
	22	$cm'm'$	22	$cm'm'$	cm^-m^-	$cm'm'$	$cmm[2]_4$	$c22'2'$	$cmm/p2$

Table 1.2.17.3 (*cont.*)

	1	18	19	20	21	22	23	24	25
	23	$pmm2$	52			pmm			
	24	$pmg2$	53			pmg			
	25	$pgg2$	54			pgg			
	26	$cmm2$	55			cmm			
	27	$pm1'$	66			$pm1'$			
	28	p'_bm	7	$pm+t'$	$pm+t^-$	$p_{2b}m$	$pm[2]_3$	$b12$	$pm/pm(m)$
	29	$pg1'$	67			$pg1'$			
	30	p'_bg	8	$pg+t'$	$pg+t^-$	$p_{2b}m'$	$pm[2]_1$	$b12_1$	pm/pg
	31	p'_b1m	9	$pm+m'$	$pm+m^-$	$p_{2a}m$	$pm[2]_5$	$b'1m$	$pm/pm(m')$
	32	p'_cm	11	$pm+g'$	$pm+g^-$	c_pm	$cm[2]_3$	$n12$	cm/pm
	33	p'_b1g	10	$pg+g'$	$pg+g^-$	$p_{2a}g$	$pg[2]_2$	$b2_11$	pg/pg
	34	p'_cg	12	$pg+m'$	$pg+m^-$	c_pm'	$cm[2]_2$	$n12_1$	cm/pg
	35	$cm1'$	68			$cm1'$			
	36	$c'm$	13	$cm+m'$	$cm+m^-$	p_cm	$pm[2]_2$	$ca12$	pm/cm
	37	$pmm21'$	69			$pmm1'$			
	38	p'_bgm	25	$pg, m+m'$	$pg, m+m^-$	$p_{2a}mm'$	$pmm[2]_4$	$a2_12$	pmm/pmg
	39	p'_cgg	29	$pg+m', g+m'$	$pg+m^-, g+m^-$	$c_pm'm'$	$cmm[2]_1$	$n2_12_1$	cmm/pgg
	40	$pmg21'$	70			$pmg1'$			
	41	p'_bmm	23	$pm, m+m'$	$pm, m+m^-$	$p_{2a}mm$	$pmm[2]_1$	$a22$	pmm/pmm
	42	p'_cmg	28	$pm+g', g+m'$	$pm+g^-, g+m^-$	c_pmm'	$cmm[2]_3$	$n22_1$	cmm/pmg
	43	p'_bgg	26	$pg, g+g'$	$pg, g+g^-$	$p_{2b}m'g$	$pmg[2]_3$	$a2_12_1$	pmg/pgg
	44	$pgg21'$	71			$pgg1'$			
	45	p'_bmg	24	$pm, g+g'$	$pm, g+g^-$	$p_{2b}mg$	$pmg[2]_1$	$b2_12$	pmg/pmg
	46	p'_cmm	27	$pm+g', m+g'$	$pm+g^-, m+g^-$	c_pmm	$cmm[2]_5$	$n22$	cmm/pmm
	47	$cmm21'$	72			$cmm1'$			
	48	$c'mm$	30	$cm+m', m+m'$	$cm+m^-, m+m^-$	p_cmm	$pmm[2]_3$	$ca22$	pmm/cmm
Tetragonal/square	49	$p4$	56			$p4$			
	50	$p4'$	31	$p4'$	$p4^-$	$p4'$	$p4[2]_2$	$4'11$	$p4/p2$
	51	$p41'$	73			$p41'$			
	52	p'_c4	32	$p4t'$	$p4t^-$	p_p4	$p4[2]_1$	$4/n11$	$p4/p4$
	53	$p4m'm'$	35	$p4m'm'$	$p4m^-m^-$	$p4m'$	$pm4[2]_2$	$42'2'$	$p4m/p4$
	54	$p4g'm'$	38	$p4g'm'$	$p4g^-m^-$	$p4g'$	$p4g[2]_1$	$42'_12'$	$p4g/p4$
	55	$p4mm$	57			$p4m$			
	56	$p4gm$	58			$p4g$			
	57	$p4'm'm$	34	$p4'm'm$	$p4^-m^-m$	$p4'm'$	$p4m[2]_3$	$4'2'2$	$p4m/cmm$
	58	$p4'g'm$	37	$p4'g'm$	$p4^-g^-m$	$p4'g'$	$p4g[2]_2$	$4'2'_12$	$p4g/cmm$
	59	$p4'mm'$	33	$p4'mm'$	$p4^-mm^-$	$p4'm$	$p4m[2]_4$	$4'22'$	$p4m/pmm$
	60	$p4'gm'$	36	$p4'gm'$	$p4^-gm^-$	$p4'g$	$p4g[2]_3$	$4'2_12'$	$p4g/pgg$
	61	$p4mm1'$	74			$p4m1'$			
	62	p'_c4gm	40	$p4g+m', m+m'$	$p4g+m^-, m+m^-$	p_p4m'	$p4m[2]_1$	$4/n2_12$	$p4m/p4g$
	63	$p4gm1'$	75			$p4g1'$			
	64	p'_c4mm	39	$p4m+g', m+m'$	$p4m+g^-, m+m^-$	p_p4m	$p4m[2]_5$	$4/n22$	$p4m/p4m$
Trigonal/hexagonal	65	$p3$	59			$p3$			
	66	$p6'$	43	$p6'$	$p6^-$	$p6'$	$p6[2]$	$6'$	$p6/p3$
	67	$p3m'$	41	$p3m'1$	$p3m^-1$	$p3m'1$	$p3m1[2]$	$312'$	$p3m1/p3$
	68	$p31m'$	42	$p31m'$	$p31m^-$	$p31m'$	$p31m[2]$	$32'1$	$p31m/p3$
	69	$p3m$	60			$p3m1$			
	70	$p31m$	61			$p31m$			
	71	$p6'm'm$	44	$p6'm'm$	$p6^-m^-m$	$p6'm'$	$p6m[2]_1$	$6'22'$	$p6m/p31m$
	72	$p6'mm'$	45	$p6'mm'$	$p6^-mm^-$	$p6'm$	$p6m[2]_2$	$6'2'2$	$p6m/p3m1$
Hexagonal/hexagonal	73	$p6$	62			$p6$			
	74	$p3'$	76			$p31'$			
	75	$p61'$	79			$p61'$			
	76	$p6m'm'$	46	$p6m'm'$	$p6m^-m^-$	$p6m'$	$p6m[2]_3$	$62'2'$	$p6m/p6$
	77	$p6mm$	63			$p6m$			
	78	$p3'm$	77			$p3m11'$			
	79	$p3'1m$	78			$p31m1'$			
	80	$p6mm1'$	80			$p6m1'$			

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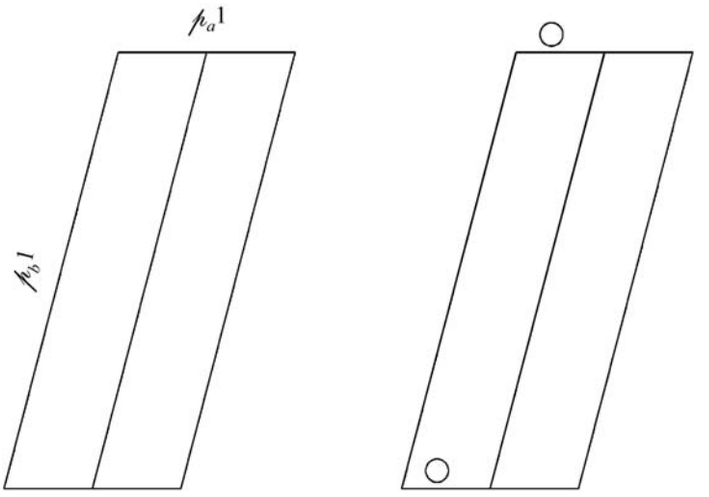
$p1$ 1 Oblique

No. 1 $p1$ Patterson symmetry $p2$



Origin arbitrary

Asymmetric unit $0 \leq x \leq 1$

Symmetry operations

(1) 1
$(1|0,0)$

Generators selected (1); $t(1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
1 a 1	(1) x,y	no conditions

Symmetry of special projections

Along [10] 1

Origin at $x,0$

Along [01] $p1$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y$

Maximal non-isotypic subgroups

I none
IIa none
IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $p1$ ($\mathbf{a}' = 2\mathbf{a}$) (1)

Minimal non-isotypic supergroups

I [2] $p211$ (2); [2] $p1m1$ (3); [2] $p11m$ (4); [2] $p11g$ (5)
II none

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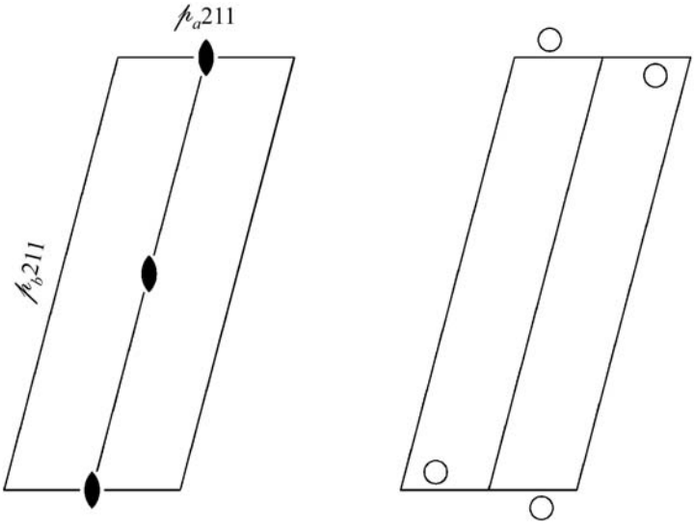
Oblique 2 $\not p211$

Patterson symmetry $\not p211$ $\not p211$ No. 2



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0$
$(1|0,0)$ $(2|0,0)$

Generators selected (1); $t(1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y	(2) $\bar{x},\bar{y}$	no conditions
					Special: no extra conditions
1	b	2	$\frac{1}{2},0$		
1	a	2	$0,0$		

Symmetry of special projections

Along [10] m
Origin at $x,0$

Along [01] $\not pm$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $\not p211$ ($\mathbf{a}' = 2\mathbf{a}$) (2)

Minimal non-isotypic supergroups

I [2] $\not p2mm$ (6); [2] $\not p2mg$ (7)
II none

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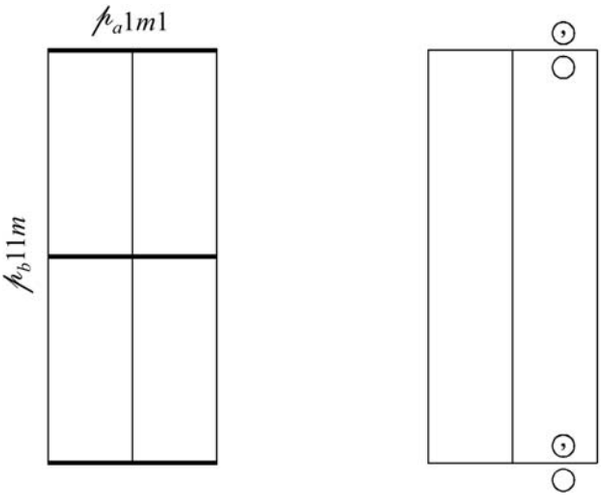
$\not p\,1\,m\,1$ m Rectangular

No. 3 $\not p\,1\,m\,1$ Patterson symmetry $\not p\,2\,m\,m$



Origin on m

Asymmetric unit $0 \le x \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0)$ (2) m $0,y$ $(m_x|0,0)$

Generators selected (1); $t(1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y	(2) $\bar{x},y$	no conditions
					Special: no extra conditions
1	b	$.m.$	$\frac{1}{2},y$		
1	a	$.m.$	$0,y$		

Symmetry of special projections

Along [10] 1
Origin at $x,0$

Along [01] $\not p\,m$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p\,1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $\not p\,1\,m\,1$ ($\mathbf{a}' = 2\mathbf{a}$) (3)

Minimal non-isotypic supergroups

I [2] $\not p\,2\,m\,m$ (6); [2] $\not p\,2\,m\,g$ (7)
II none

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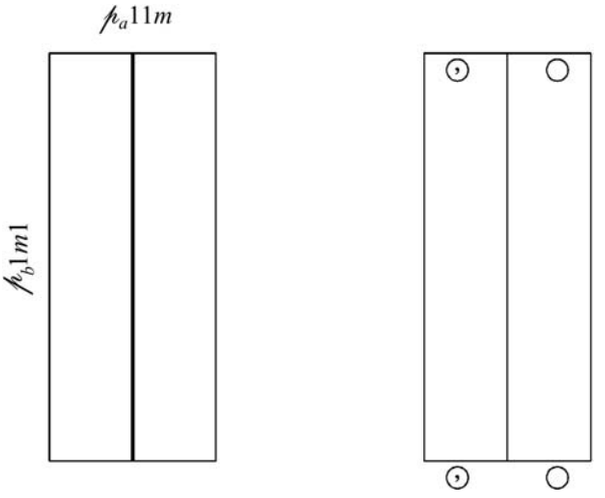
Rectangular m $\not p 11m$

Patterson symmetry $\not p 2mm$ $\not p 11m$ No. 4



Origin on m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y$

Symmetry operations

(1) 1 (2) m $x,0$
$(1|0,0)$ $(m_y|0,0)$

Generators selected (1); $t(1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 b 1	(1) x,y	(2) $x,\bar{y}$	no conditions
			Special: no extra conditions
1 a $..m$	$x,0$		

Symmetry of special projections

Along [10] m
$\mathbf{a}' = \mathbf{a}$
Origin at $x,0$

Along [01] $\not p 1$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p 1$ (1) 1

IIa none

IIb [2] $\not p 1\,1\,g$ ($\mathbf{a}' = 2\mathbf{a}$) (5)

Maximal isotypic subgroups of lowest index

IIc [2] $\not p 1\,1\,m$ ($\mathbf{a}' = 2\mathbf{a}$) (4)

Minimal non-isotypic supergroups

I [2] $\not p 2mm$ (6)

II none

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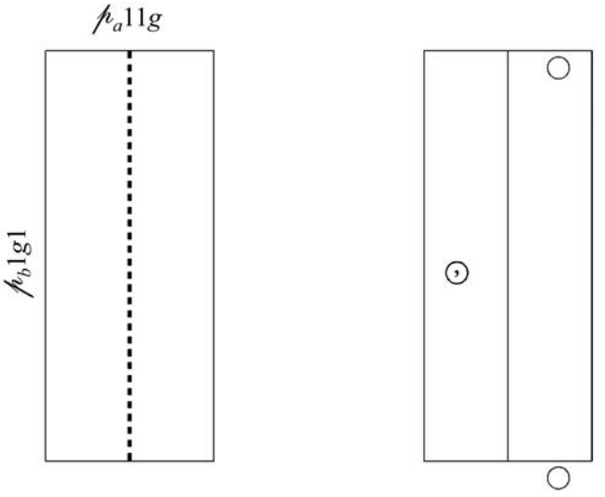
$\not p 1\,1\,g$ m Rectangular

No. 5 $\not p 1\,1\,g$ Patterson symmetry $\not p 2\,m\,m$



Origin on g

Asymmetric unit $0 \le x \le 1; \quad 0 \le y$

Symmetry operations

(1) 1 (2) g $x,0$
$(1|0,0)$ $(m_y|\frac{1}{2},0)$

Generators selected (1); $t(1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y (2) $x+\frac{1}{2},\bar{y}$	h : $h=2n$

Symmetry of special projections

Along [10] m

Origin at $x,0$

Along [01] $\not p 1$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p 1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $\not p 1\,1\,g$ ($\mathbf{a}' = 3\mathbf{a}$) (5)

Minimal non-isotypic supergroups

I [2] $\not p 2\,m\,g$ (7)

II [2] $\not p 1\,1\,m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (4)

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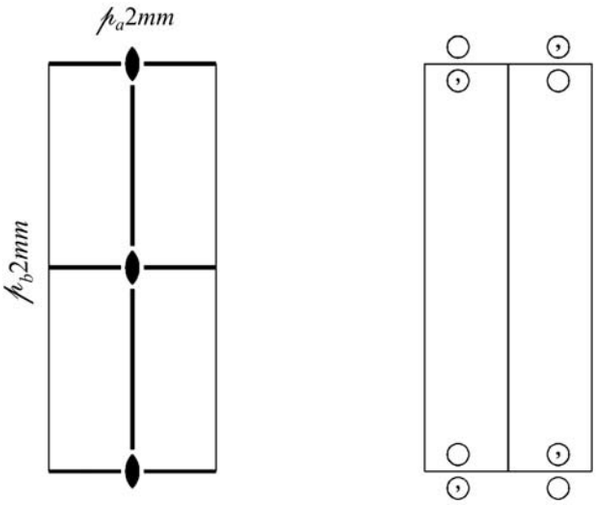
Rectangular $2mm$ $\not p2mm$

Patterson symmetry $\not p2mm$ $\not p2mm$ No. 6



Origin at $2mm$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $0,y$ (4) m $x,0$
$(1|0,0)$ $(2|0,0)$ $(m_x|0,0)$ $(m_y|0,0)$

Generators selected (1); $t(1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	f	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$	General: no conditions
2	e	$.m.$	$\frac{1}{2},y$	$\frac{1}{2},\bar{y}$			Special: no extra conditions
2	d	$.m.$	$0,y$	$0,\bar{y}$			
2	c	$..m$	$x,0$	$\bar{x},0$			
1	b	$2\,m\,m$	$\frac{1}{2},0$				
1	a	$2\,m\,m$	$0,0$				

Symmetry of special projections

Along [10] m
Origin at $x,0$

Along [01] $\not pm$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p1\,1\,m$ (4) 1; 4
[2] $\not p1\,m\,1$ (3) 1; 3
[2] $\not p2\,1\,1$ (2) 1; 2

IIa none

IIb [2] $\not p2mg$ ($\mathbf{a}' = 2\mathbf{a}$) (7)

Maximal isotypic subgroups of lowest index

IIc [2] $\not p2mm$ ($\mathbf{a}' = 2\mathbf{a}$) (6)

Minimal non-isotypic supergroups

I none

II none

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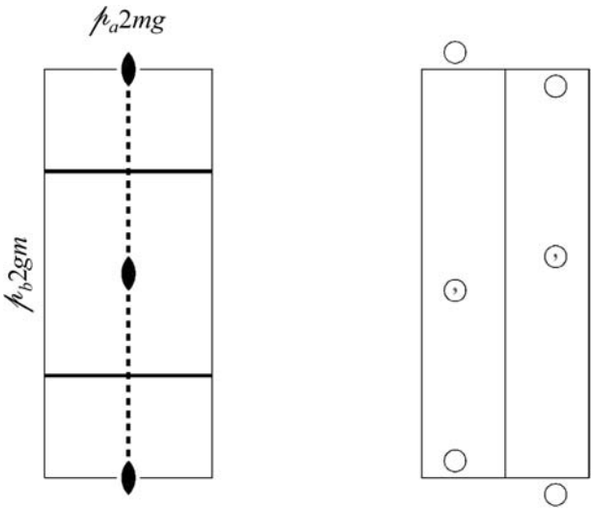
$\not p 2mg$ $2mm$ Rectangular

No. 7 $\not p 2mg$

Patterson symmetry $\not p 2mm$



Origin at $2\,1\,g$

Asymmetric unit $0 \le x \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $\frac{1}{4},y$ (4) g $x,0$
$(1|0,0)$ $(2|0,0)$ $(m_x|\frac{1}{2},0)$ $(m_y|\frac{1}{2},0)$

Generators selected (1); $t(1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x}+\frac{1}{2},y$	(4) $x+\frac{1}{2},\bar{y}$	h : $h=2n$
							Special: no extra conditions
2	b	$.m.$	$\frac{1}{4},y$	$\frac{3}{4},\bar{y}$			
2	a	$2..$	$0,0$	$\frac{1}{2},0$			

Symmetry of special projections

Along [10] m

Origin at $x,0$

Along [01] $\not p m$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y$

Maximal non-isotypic subgroups

I [2] $\not p 1\,1\,g$ (5) 1; 4
[2] $\not p 1\,m\,1$ (3) 1; 3
[2] $\not p 2\,1\,1$ (2) 1; 2

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $\not p 2mg$ ($\mathbf{a}' = 3\mathbf{a}$) (7)

Minimal non-isotypic supergroups

I none

II [2] $\not p 2mm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (6)

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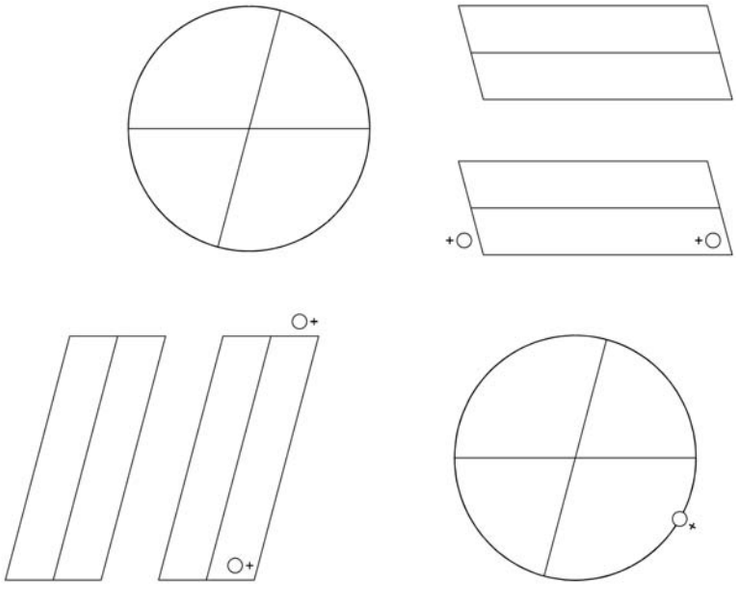
$p1$ 1 Triclinic

No. 1 $p1$ Patterson symmetry $p\bar{1}$



Origin arbitrary

Asymmetric unit $0 \leq z \leq 1$

Symmetry operations

(1) 1
$(1|0,0,0)$

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Generators selected (1); $t(0,0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
1 a 1	(1) x,y,z	no conditions

Symmetry of special projections

Along [001] 1	Along [100] $\not{p}1$	Along [010] $\not{p}1$
	$\mathbf{a}' = \mathbf{c}_p$	$\mathbf{a}' = \mathbf{c}_p$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I none

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}1$ ($\mathbf{c}' = 2\mathbf{c}$) (1)

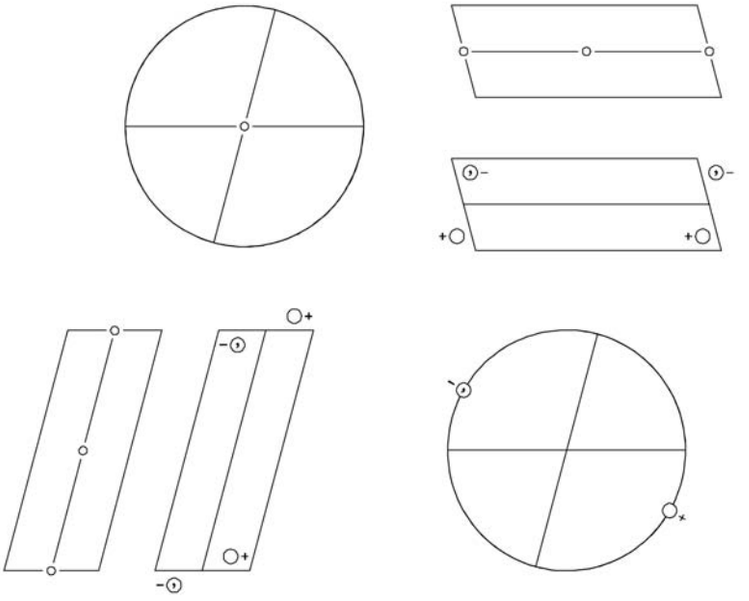
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}\bar{1}$ (2); [2] $\not{p}2\,1\,1$ (3); [2] $\not{p}m\,1\,1$ (4); [2] $\not{p}c\,1\,1$ (5); [2] $\not{p}1\,1\,2$ (8); [2] $\not{p}1\,1\,2_1$ (9); [2] $\not{p}1\,1\,m$ (10); [3] $\not{p}3$ (42); [3] $\not{p}3_1$ (43); [3] $\not{p}3_2$ (44)

II none

$p\bar{1}$ $\bar{1}$ Triclinic

No. 2 $p\bar{1}$ Patterson symmetry $p\bar{1}$



Origin at $\bar{1}$

Asymmetric unit $0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 (2) $\bar{1}$ 0,0,0
(1|0,0,0) ($\bar{1}$|0,0,0)

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$	no conditions
					Special: no extra conditions
1	b	$\bar{1}$	$0,0,\frac{1}{2}$		
1	a	$\bar{1}$	$0,0,0$		

Symmetry of special projections

Along [001] 2 1 1	Along [100] $\not{p}$ 2 1 1	Along [010] $\not{p}$ 2 1 1
Origin at $0,0,z$	$\mathbf{a}' = \mathbf{c}_p$ Origin at $x,0,0$	$\mathbf{a}' = \mathbf{c}_p$ Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}$ 1 (1) 1

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{1}$ ($\mathbf{c}' = 2\mathbf{c}$) (2)

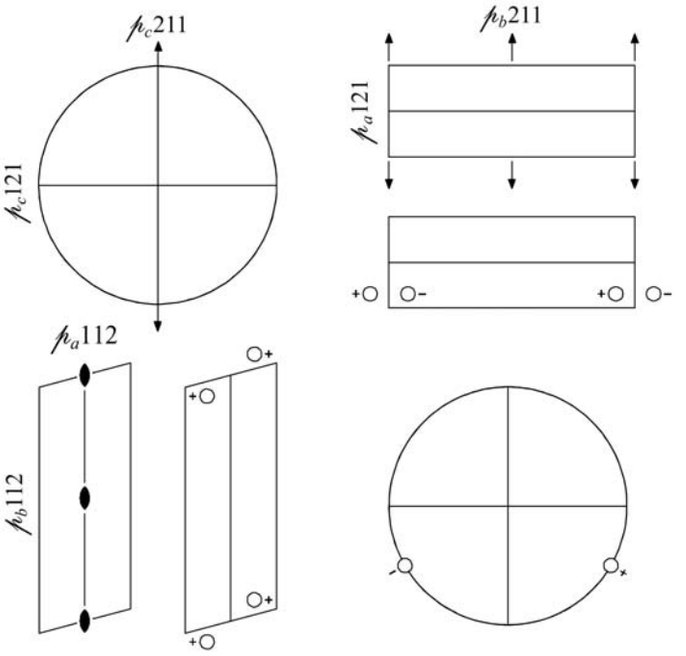
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}$ 2/m 1 1 (6); [2] $\not{p}$ 2/c 1 1 (7); [2] $\not{p}$ 1 1 2/m (11); [2] $\not{p}$ 1 1 $2_1/m$ (12); [3] $\not{p}\bar{3}$ (45)

II none

$p211$ 2 Monoclinic/Oblique

No. 3 $p211$ Patterson symmetry $p2/m11$



Origin on 2

Asymmetric unit $0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $x,0,0$ $(2_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	no conditions
					Special: no extra conditions
1	b	2	$x,0,\frac{1}{2}$		
1	a	2	$x,0,0$		

Symmetry of special projections

Along [001] $1\,1\,m$
Origin at $0,0,z$

Along [100] $\not{p}2\,1\,1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}1\,m\,1$
$\mathbf{a}' = \mathbf{c}_p$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}2\,1\,1$ ($\mathbf{c}' = 2\mathbf{c}$) (3)

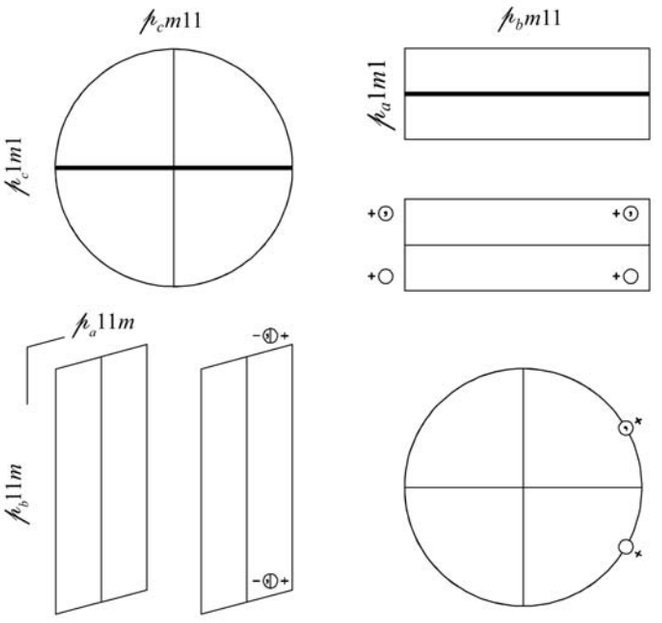
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}2/m\,1\,1$ (6); [2] $\not{p}2/c\,1\,1$ (7); [2] $\not{p}2\,2\,2$ (13); [2] $\not{p}2\,2\,2_1$ (14); [2] $\not{p}2\,m\,m$ (18); [2] $\not{p}2\,c\,m$ (19); [3] $\not{p}3\,1\,2$ (46); [3] $\not{p}3_1\,1\,2$ (47); [3] $\not{p}3_2\,1\,2$ (48)

II none

$\not{p}m11$ m Monoclinic/Oblique

No. 4 $\not{p}m11$ Patterson symmetry $\not{p}2/m11$



Origin on mirror plane m

Asymmetric unit $0 \le x; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	b 1	(1) x,y,z	(2) $\bar{x},y,z$	no conditions
				Special: no extra conditions
1	a m	$0,y,z$		

Symmetry of special projections

Along [001] $1m1$
Origin at $0,0,z$

Along [100] $p\bar{1}11$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p\bar{1}1m$
$\mathbf{a}' = \mathbf{c}_p$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $p\bar{1}$ (1) 1

IIa none

IIb [2] $p\bar{c}11$ ($\mathbf{c}' = 2\mathbf{c}$) (5)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $p\bar{m}11$ ($\mathbf{c}' = 2\mathbf{c}$) (4)

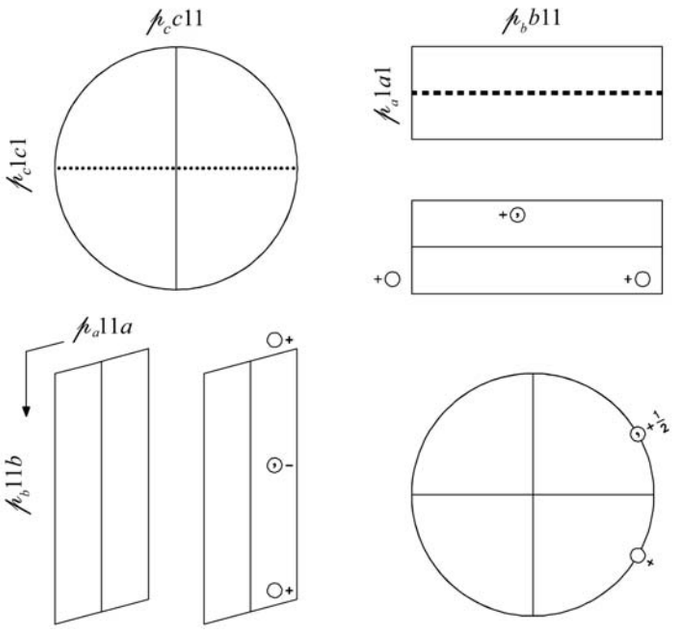
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $p\bar{2}/m11$ (6); [2] $p\bar{m}m2$ (15); [2] $p\bar{m}c2_1$ (17); [2] $p\bar{2}mm$ (18); [3] $p\bar{3}m1$ (49)

II none

$\not p c 1 1$ m Monoclinic/Oblique

No. 5 $\not p c 1 1$ Patterson symmetry $\not p 2/m\,1\,1$



Origin on glide plane c

Asymmetric unit $0 \le x; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) c $0, y, z$
$(1|0,0,0)$ $(m_x|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},y,z+\frac{1}{2}$	l : $l=2n$

Symmetry of special projections

Along [001] $1m1$
Origin at $0,0,z$

Along [100] $\not{p}1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}_p$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}c11$ ($\mathbf{c}'=3\mathbf{c}$) (5)

Minimal non-isotypic non-enantiomorphic supergroups

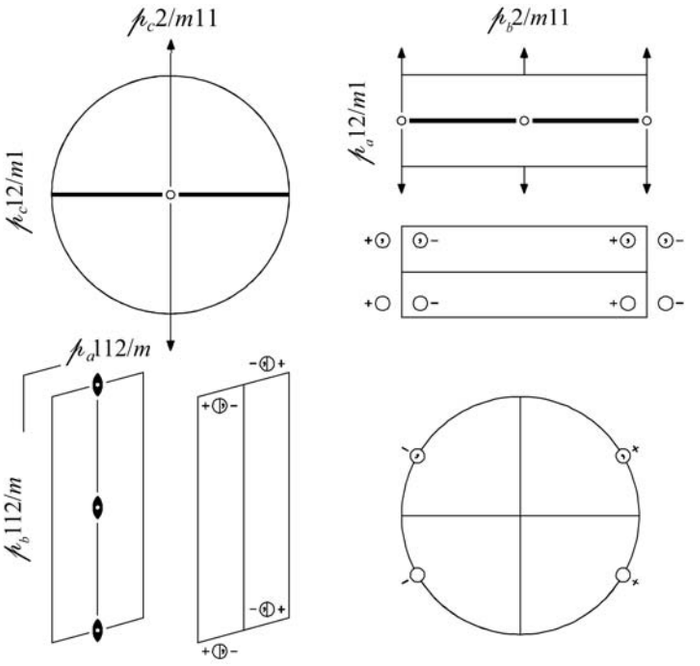
I [2] $\not{p}2/c11$ (7); [2] $\not{p}cc2$ (16); [2] $\not{p}mc2_1$ (17); [2] $\not{p}2cm$ (19); [3] $\not{p}3c1$ (50)

II [2] $\not{p}m11$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (4)

$\not p2/m11$ $2/m$ Monoclinic/Oblique

No. 6 $\not p2/m11$

Patterson symmetry $\not p2/m11$



Origin at centre $(2/m)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$
(2) $2 \quad x,0,0$ $(2_x|0,0,0)$
(3) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$
(4) $m \quad 0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x},y,z$	no conditions
							Special: no extra conditions
2	e	m	$0,y,z$	$0,\bar{y},\bar{z}$			
2	d	2	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	c	2	$x,0,0$	$\bar{x},0,0$			
1	b	$2/m$	$0,0,\frac{1}{2}$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{p}211$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}_p$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}m11$ (4) 1; 4
[2] $\not{p}211$ (3) 1; 2
[2] $\not{p}\bar{1}$ (2) 1; 3

IIa none

IIb [2] $\not{p}2/c11$ ($\mathbf{c}' = 2\mathbf{c}$) (7)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}2/m11$ ($\mathbf{c}' = 2\mathbf{c}$) (6)

Minimal non-isotypic non-enantiomorphic supergroups

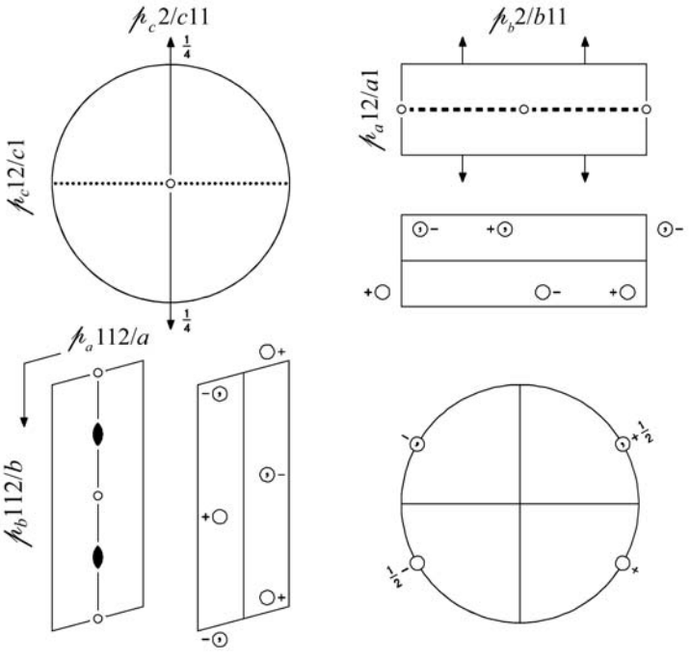
I [2] $\not{p}mmm$ (20); [2] $\not{p}mcm$ (22); [3] $\not{p}\bar{3}1m$ (51)

II none

$\not p2/c11$ $2/m$ Monoclinic/Oblique

No. 7 $\not p2/c11$

Patterson symmetry $\not p2/m11$



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 2 $x,0,\frac{1}{4}$ $(2_x|0,0,\frac{1}{2})$

(3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(4) c $0,y,z$ $(m_x|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x},y,z+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
2	b	2	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$			
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not p211$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not p2mg$
$\mathbf{a}'=\mathbf{c}_p$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not pc11$ (5) 1; 4
[2] $\not p211$ (3) 1; 2
[2] $\not p\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not p2/c11$ ($\mathbf{c}'=3\mathbf{c}$) (7)

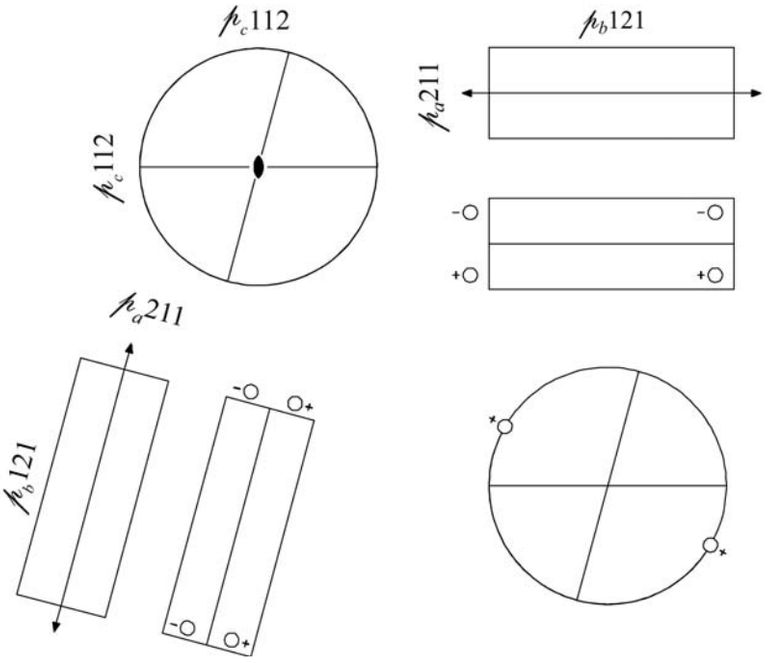
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not pccm$ (21); [2] $\not pmcm$ (22); [3] $\not p\bar{3}1c$ (52)

II [2] $\not p2/m11$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (6)

$p112$ 2 Monoclinic/Rectangular

No. 8 $p112$ Patterson symmetry $p112/m$



Origin on 2

Asymmetric unit $0 \le x; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$
$(1|0,0,0)$ $(2_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	no conditions
					Special: no extra conditions
1	a	2	$0,0,z$		

Symmetry of special projections

Along [001] 2 1 1
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1$ (1) 1

IIa none

IIb [2] $\not{p}1\,1\,2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (9)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}1\,1\,2$ ($\mathbf{c}' = 2\mathbf{c}$) (8)

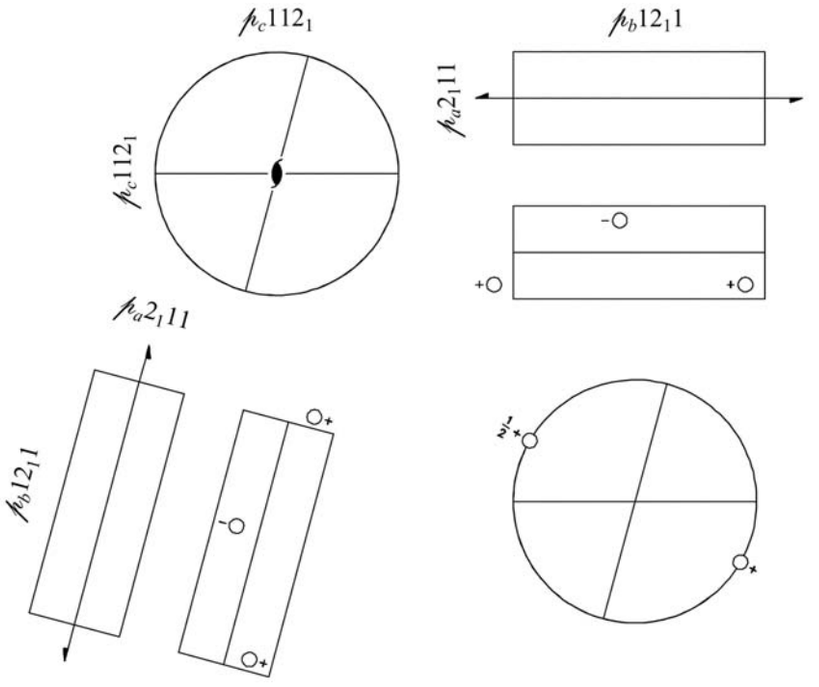
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}1\,1\,2/m$ (11); [2] $\not{p}2\,2\,2$ (13); [2] $\not{p}m\,m\,2$ (15); [2] $\not{p}c\,c\,2$ (16); [2] $\not{p}4$ (23); [2] $\not{p}4_2$ (25); [2] $\not{p}\bar{4}$ (27); [3] $\not{p}6$ (53); [3] $\not{p}6_2$ (55); [3] $\not{p}6_4$ (57)

II none

$p112_1$ 2 Monoclinic/Rectangular

No. 9 $p112_1$ Patterson symmetry $p112/m$



Origin on 2_1

Asymmetric unit $0 \le x; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$	l : $l=2n$

Symmetry of special projections

Along [001] 2 1 1
Origin at $0,0,z$

Along [100] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

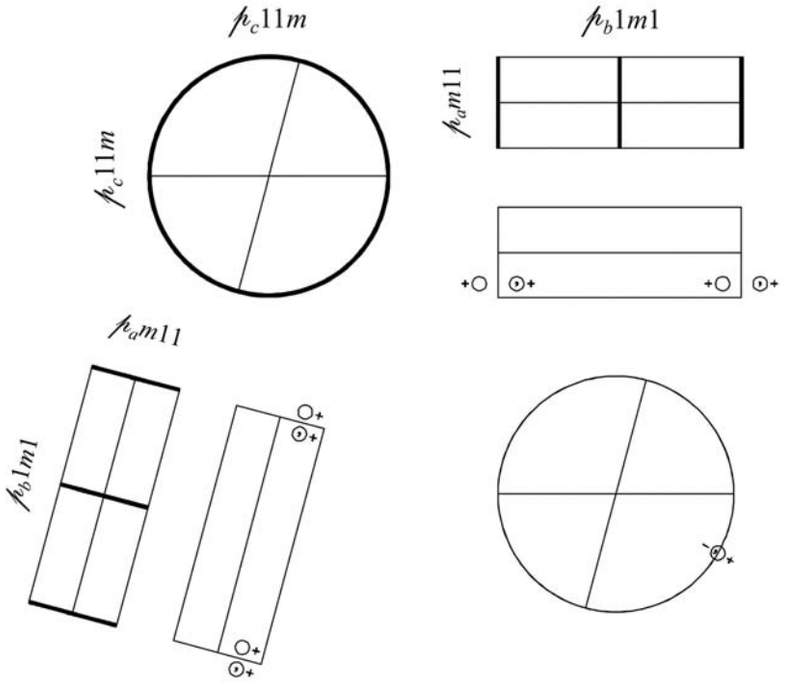
IIc [3] $\not{p}112_1$ ($\mathbf{c}'=3\mathbf{c}$) (9)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}112_1/m$ (12); [2] $\not{p}222_1$ (14); [2] $\not{p}mc2_1$ (17); [2] $\not{p}4_1$ (24); [2] $\not{p}4_3$ (26); [3] $\not{p}6_1$ (54); [3] $\not{p}6_3$ (56); [3] $\not{p}6_5$ (58)
II [2] $\not{p}112$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (8)

$\not{p}11m$ m Monoclinic/Rectangular

No. 10 $\not{p}11m$ Patterson symmetry $\not{p}112/m$



Origin on mirror plane m

Asymmetric unit $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,y,\bar{z}$	no conditions
					Special: no extra conditions
1	b	m	$x,y,\frac{1}{2}$		
1	a	m	$x,y,0$		

Symmetry of special projections

Along [001] 1	Along [100] $\not{p}1m1$	Along [010] $\not{p}1m1$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}11m$ ($\mathbf{c}' = 2\mathbf{c}$) (10)

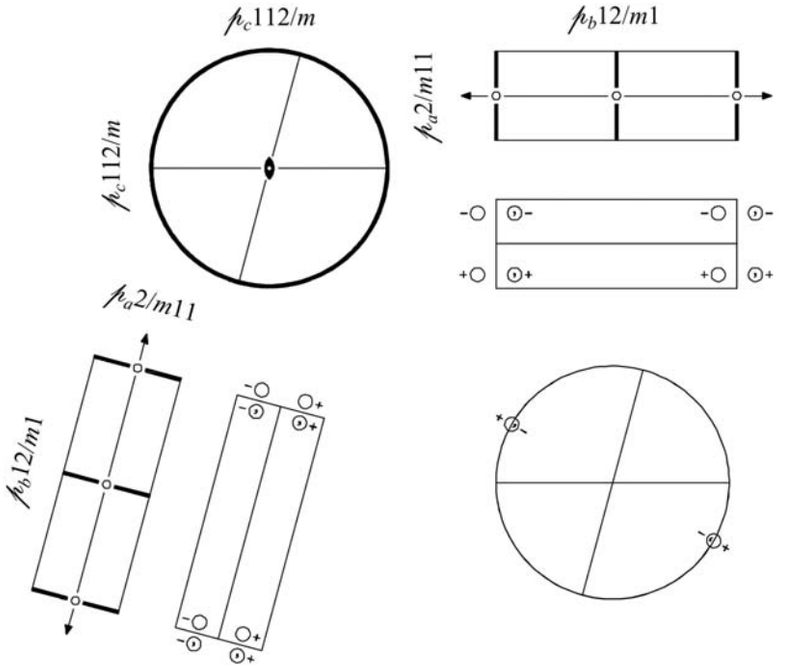
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}112/m$ (11); [2] $\not{p}112_1/m$ (12); [2] $\not{p}2mm$ (18); [2] $\not{p}2cm$ (19); [2] $\not{p}\bar{6}$ (59)

II none

$\not p 1\,1\,2/m$ $2/m$ Monoclinic/Rectangular

No. 11 $\not p 1\,1\,2/m$ Patterson symmetry $\not p 1\,1\,2/m$



Origin at centre $(2/m)$

Asymmetric unit $0 \le y;\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $0,0,z$ $(2_z|0,0,0)$ (3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$ (4) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	no conditions
							Special: no extra conditions
2	e	m	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$			
2	d	m	$x,y,0$	$\bar{x},\bar{y},0$			
2	c	2	$0,0,z$	$0,0,\bar{z}$			
1	b	$2/m$	$0,0,\frac{1}{2}$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] 2 1 1
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,m$ (10) 1; 4
[2] $\not{p}1\,1\,2$ (8) 1; 2
[2] $\not{p}\bar{1}$ (2) 1; 3

IIa none

IIb [2] $\not{p}1\,1\,2_1/m$ ($\mathbf{c}' = 2\mathbf{c}$) (12)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}1\,1\,2/m$ ($\mathbf{c}' = 2\mathbf{c}$) (11)

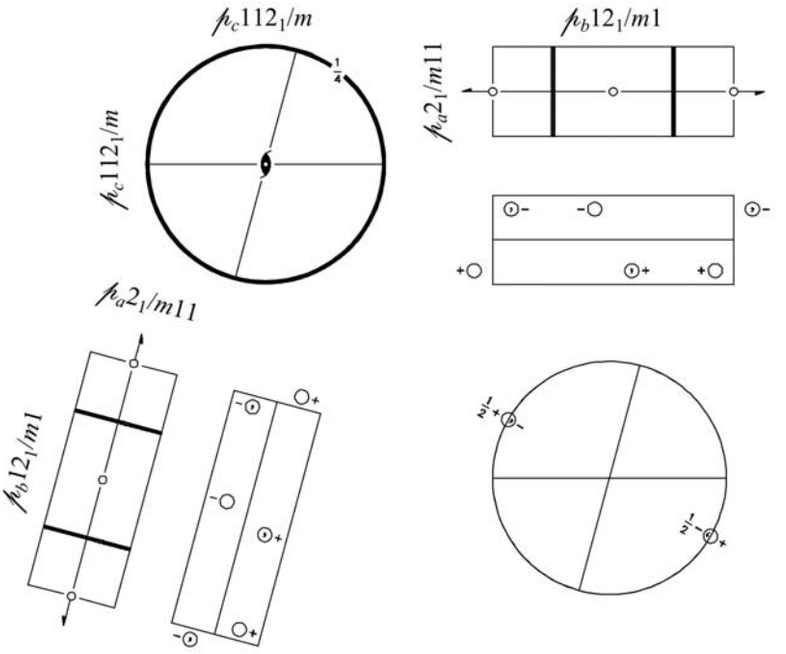
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}mmm$ (20); [2] $\not{p}ccm$ (21); [2] $\not{p}4/m$ (28); [2] $\not{p}4_2/m$ (29); [3] $\not{p}6/m$ (60)

II none

$\not p 1\,1\,2_1/m$ $2/m$ Monoclinic/Rectangular

No. 12 $\not p 1\,1\,2_1/m$ Patterson symmetry $\not p 1\,1\,2/m$



Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$ (3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$ (4) m $x,y,\frac{1}{4}$ $(m_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
2	b	m	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$			
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] 2 1 1
Origin at $0,0,z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}11m$ (10) 1; 4
[2] $\not{p}112_1$ (9) 1; 2
[2] $\not{p}\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}112_1/m$ ($\mathbf{c}'=3\mathbf{c}$) (12)

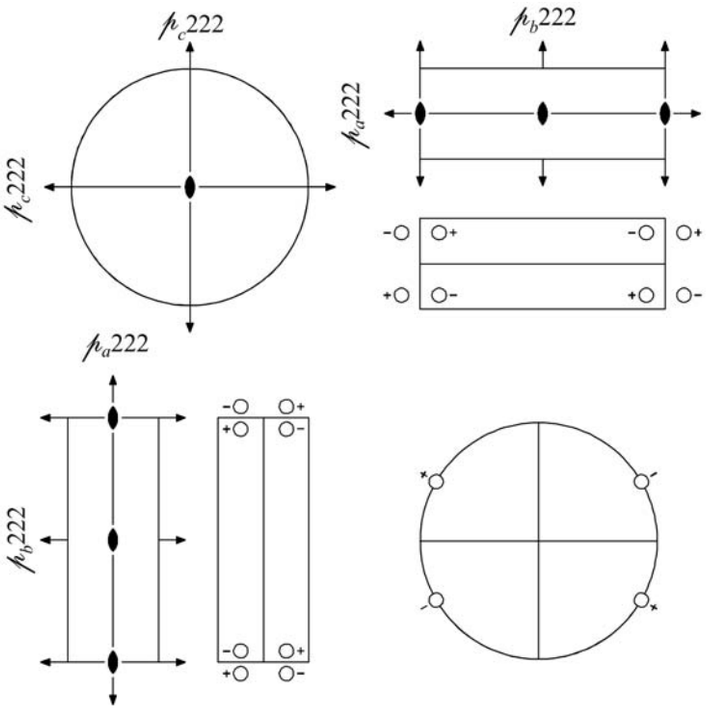
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}mcm$ (22); [3] $\not{p}6_3/m$ (61)

II [2] $\not{p}112/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (11)

$p222$ 222 Orthorhombic

No. 13 $p222$ Patterson symmetry $pmmm$



Origin at 222

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $0,0,z$ $(2_z|0,0,0)$ (3) 2 $0,y,0$ $(2_y|0,0,0)$ (4) 2 $x,0,0$ $(2_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
							Special: no extra conditions
2	g	. . 2	$0,0,z$	$0,0,\bar{z}$			
2	f	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	e	. 2 .	$0,y,0$	$0,\bar{y},0$			
2	d	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	c	2 . .	$x,0,0$	$\bar{x},0,0$			
1	b	2 2 2	$0,0,\frac{1}{2}$				
1	a	2 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not P2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not P2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not P112$ (8) 1; 2
[2] $\not P121$ ($\not P211$, 3) 1; 3
[2] $\not P211$ (3) 1; 4

IIa none

IIb [2] $\not P222_1$ ($\mathbf{c}' = 2\mathbf{c}$) (14)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not P222$ ($\mathbf{c}' = 2\mathbf{c}$) (13)

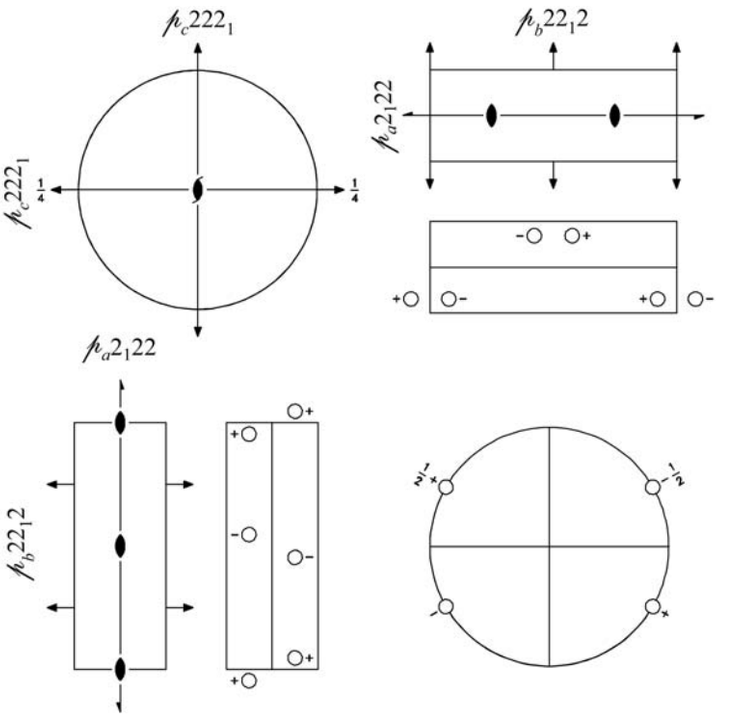
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not Pmmm$ (20); [2] $\not Pccm$ (21); [2] $\not P422$ (30); [2] $\not P4_222$ (32); [2] $\not P\bar{4}2m$ (37); [2] $\not P\bar{4}2c$ (38); [3] $\not P622$ (62); [3] $\not P6_222$ (64); [3] $\not P6_422$ (66)

II none

$p222_1$ 222 Orthorhombic

No. 14 $p222_1$ Patterson symmetry $pmmm$



Origin at 212_1

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$ (3) 2 $0,y,\frac{1}{4}$ $(2_y|0,0,\frac{1}{2})$ (4) 2 $x,0,0$ $(2_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$	General:
							l : $l=2n$
							Special: no extra conditions
2	b	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			
2	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not P2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not P2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $0,y,\frac{1}{4}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not P112_1$ (9) 1; 2
[2] $\not P121$ ($\not P211$, 3) 1; 3
[2] $\not P211$ (3) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not P222_1$ ($\mathbf{c}'=3\mathbf{c}$) (14)

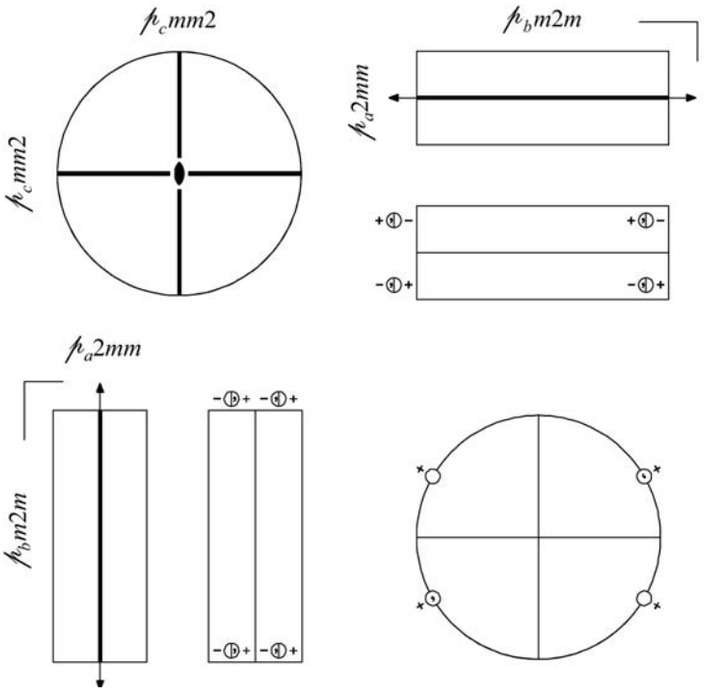
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not Pmcm$ (22); [2] $\not P4_122$ (31); [2] $\not P4_322$ (33); [3] $\not P6_122$ (63); [3] $\not P6_322$ (65); [3] $\not P6_522$ (67)

II [2] $\not P222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (13)

$\not{p}mm2$ $mm2$ Orthorhombic

No. 15 $\not{p}mm2$ Patterson symmetry $\not{p}mmm$



Origin on $mm2$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$
(2) 2 $0,0,z$ $(2_z|0,0,0)$
(3) m $x,0,z$ $(m_y|0,0,0)$
(4) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	no conditions
							Special: no extra conditions
2	c	m . .	$0,y,z$	$0,\bar{y},z$			
2	b	. m .	$x,0,z$	$\bar{x},0,z$			
1	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,2$ (8) 1; 2
[2] $\not{p}1\,m\,1$ ($\not{p}m\,1\,1$, 4) 1; 3
[2] $\not{p}m\,1\,1$ (4) 1; 4

IIa none

IIb [2] $\not{p}mc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (17); [2] $\not{p}cm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}mc2_1$, 17); [2] $\not{p}cc2$ ($\mathbf{c}' = 2\mathbf{c}$) (16)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}mm2$ ($\mathbf{c}' = 2\mathbf{c}$) (15)

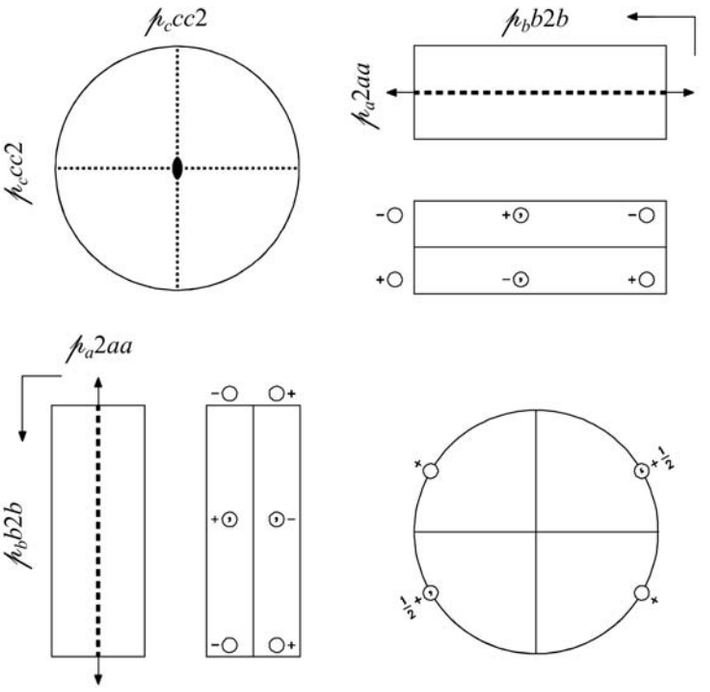
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}mmm$ (20); [2] $\not{p}4mm$ (34); [2] $\not{p}4_2cm$ (35); [2] $\not{p}\bar{4}2m$ (37); [3] $\not{p}6mm$ (68)

II none

$\not{p}cc2$ $mm2$ Orthorhombic

No. 16 $\not{p}cc2$ Patterson symmetry $\not{p}mmm$



Origin on $cc2$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) $2 \quad 0,0,z$ $(2_z|0,0,0)$ (3) $c \quad x,0,z$ $(m_y|0,0,\frac{1}{2})$ (4) $c \quad 0,y,z$ $(m_x|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 b 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	General: l : $l=2n$
2 a . . 2	$0,0,z$	$0,0,z+\frac{1}{2}$			Special: no extra conditions

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}112$ (8) 1; 2
[2] $\not{p}1c1$ ($\not{p}c11$, 5) 1; 3
[2] $\not{p}c11$ (5) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}cc2$ ($\mathbf{c}'=3\mathbf{c}$) (16)

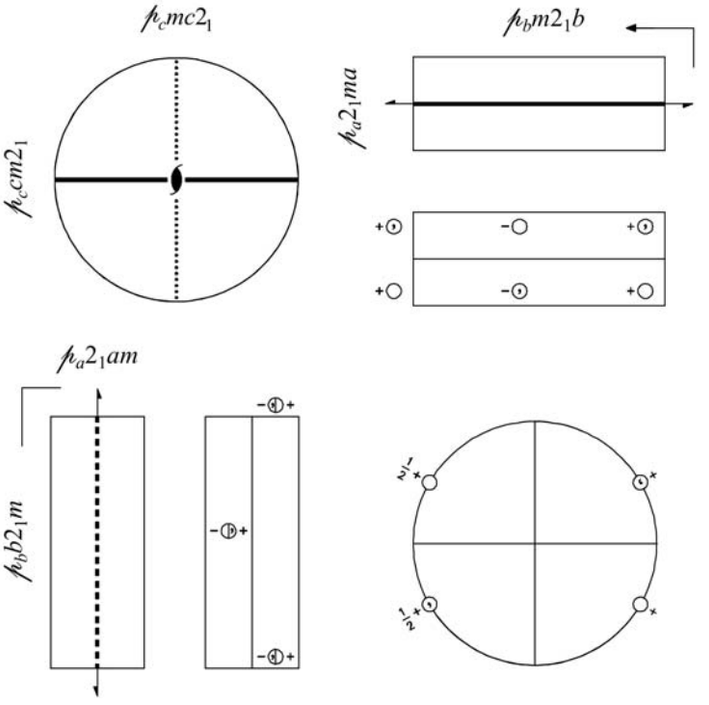
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}ccm$ (21); [2] $\not{p}4_2cm$ (35); [2] $\not{p}4cc$ (36); [2] $\not{p}\bar{4}2c$ (38); [3] $\not{p}6cc$ (69)

II [2] $\not{p}mm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (15)

$\not p m c 2_1$ $mm2$ Orthorhombic

No. 17 $\not p m c 2_1$ Patterson symmetry $\not p m m m$



Origin on $mc2_1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(3) c $x,0,z$ $(m_y|0,0,\frac{1}{2})$

(4) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 b 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z$	General: l : $l=2n$
		Special: no extra conditions
2 a m . .	$0,y,z$ $0,\bar{y},z+\frac{1}{2}$	

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,2_1$ (9) 1; 2
[2] $\not{p}1\,c\,1$ ($\not{p}c\,1\,1$, 5) 1; 3
[2] $\not{p}m\,1\,1$ (4) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}mc2_1$ ($\mathbf{c}'=3\mathbf{c}$) (17)

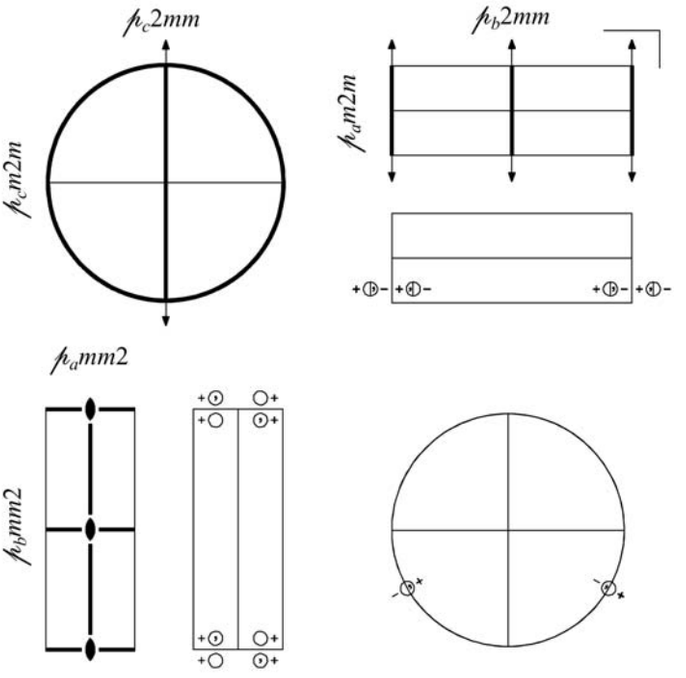
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}mcm$ (22); [3] $\not{p}6_3mc$ (70)

II [2] $\not{p}mm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (15)

$\not p2mm$ $2mm$ Orthorhombic

No. 18 $\not p2mm$ Patterson symmetry $\not pmmm$



Origin on $2mm$

Asymmetric unit $0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$
(2) $2 \quad x,0,0$ $(2_x|0,0,0)$
(3) $m \quad x,y,0$ $(m_z|0,0,0)$
(4) $m \quad x,0,z$ $(m_y|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $x,y,\bar{z}$	(4) $x,\bar{y},z$	no conditions
							Special: no extra conditions
2	e	. m .	$x,0,z$	$x,0,\bar{z}$			
2	d	. . m	$x,y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$			
2	c	. . m	$x,y,0$	$x,\bar{y},0$			
1	b	2 m m	$x,0,\frac{1}{2}$				
1	a	2 m m	$x,0,0$				

Symmetry of special projections

Along [001] 1 1 m
Origin at $0,0,z$

Along [100] $\not m2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not m1m1$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not m1\,1\,m$ (10) 1; 3
[2] $\not m1\,m\,1$ ($\not mm\,1\,1$, 4) 1; 4
[2] $\not m2\,1\,1$ (3) 1; 2

IIa none

IIb [2] $\not m2\,c\,m$ ($\mathbf{c}' = 2\mathbf{c}$) (19)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not m2\,m\,m$ ($\mathbf{c}' = 2\mathbf{c}$) (18)

Minimal non-isotypic non-enantiomorphic supergroups

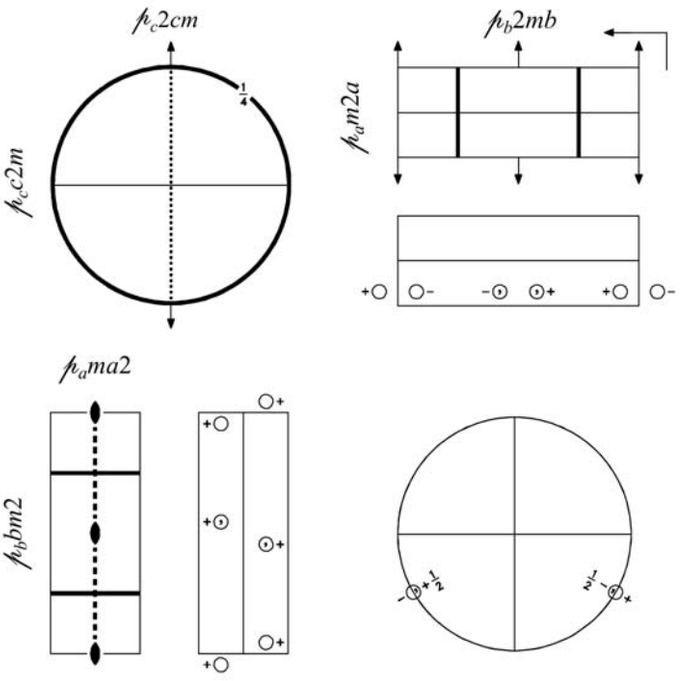
I [2] $\not mmmm$ (20); [2] $\not mcm$ (22); [3] $\not m\bar{6}m2$ (71)

II none

$\not p2cm$ $2mm$ Orthorhombic

No. 19 $\not p2cm$

Patterson symmetry $\not pmmm$



Origin on $2c1$

Asymmetric unit $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $x,0,0$ $(2_x|0,0,0)$ (3) c $x,0,z$ $(m_y|0,0,\frac{1}{2})$ (4) m $x,y,\frac{1}{4}$ $(m_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $x,y,\bar{z}+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
2	b	. . m	$x,y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$			
2	a	2 . .	$x,0,0$	$x,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] 1 1 m	Along [100] $\not{p}2mg$	Along [010] $\not{p}1m1$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}1\,1\,m$ (10)	1; 4
	[2] $\not{p}1\,c\,1$ ($\not{p}c\,1\,1$, 5)	1; 3
	[2] $\not{p}2\,1\,1$ (3)	1; 2
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}2cm$ ($\mathbf{c}'=3\mathbf{c}$) (19)

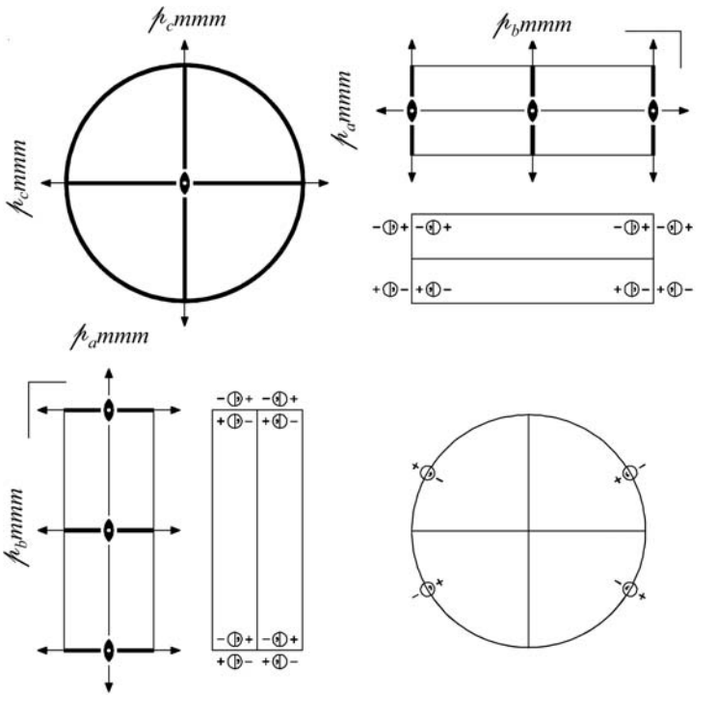
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}ccm$ (21); [2] $\not{p}mcm$ (22); [3] $\not{p}\bar{6}c2$ (72)

II [2] $\not{p}2mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (18)

$\not p mmm$ mmm Orthorhombic

No. 20 $\not p 2/m2/m2/m$ Patterson symmetry $\not p mmm$



Origin at centre (mmm)

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,0,z$ $(2_z|0,0,0)$

(3) $2 \quad 0,y,0$ $(2_y|0,0,0)$

(4) $2 \quad x,0,0$ $(2_x|0,0,0)$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$ $(m_z|0,0,0)$

(7) $m \quad x,0,z$ $(m_y|0,0,0)$

(8) $m \quad 0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	no conditions
							Special: no extra conditions
4	k	. . m	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	
4	j	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	
4	i	. m .	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	
4	h	m . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	
2	g	$m\,m\,2$	$0,0,z$	$0,0,\bar{z}$			
2	f	$m\,2\,m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	e	$m\,2\,m$	$0,y,0$	$0,\bar{y},0$			
2	d	$2\,m\,m$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	c	$2\,m\,m$	$x,0,0$	$\bar{x},0,0$			
1	b	$m\,m\,m$	$0,0,\frac{1}{2}$				
1	a	$m\,m\,m$	$0,0,0$				

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}m2m$ ($\not{p}2mm$, 18) 1; 3; 6; 8
[2] $\not{p}2mm$ (18) 1; 4; 6; 7
[2] $\not{p}mm2$ (15) 1; 2; 7; 8
[2] $\not{p}222$ (13) 1; 2; 3; 4
[2] $\not{p}112/m$ (11) 1; 2; 5; 6
[2] $\not{p}12/m1$ ($\not{p}2/m11$, 6) 1; 3; 5; 7
[2] $\not{p}2/m11$ (6) 1; 4; 5; 8

IIa none

IIb [2] $\not{p}cmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}mcm$, 22); [2] $\not{p}mcm$ ($\mathbf{c}' = 2\mathbf{c}$) (22); [2] $\not{p}ccm$ ($\mathbf{c}' = 2\mathbf{c}$) (21)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}mmm$ ($\mathbf{c}' = 2\mathbf{c}$) (20)

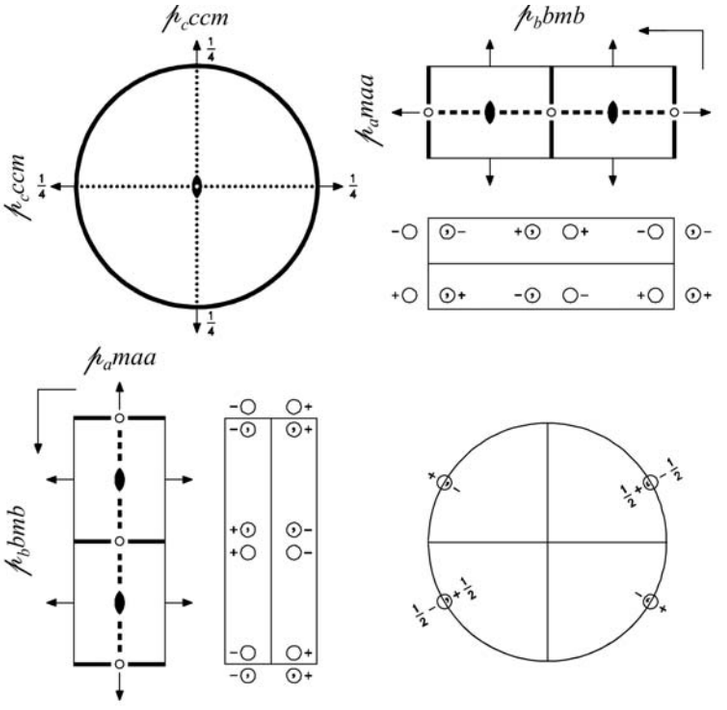
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}4/mmm$ (39); [2] $\not{p}4_2/mmc$ (41); [3] $\not{p}6/mmm$ (73)

II none

$\not p ccm$ mmm Orthorhombic

No. 21 $\not p 2/c2/c2/m$ Patterson symmetry $\not p mmm$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,0,z$ $(2_z|0,0,0)$

(3) $2 \quad 0,y,\frac{1}{4}$ $(2_y|0,0,\frac{1}{2})$

(4) $2 \quad x,0,\frac{1}{4}$ $(2_x|0,0,\frac{1}{2})$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$ $(m_z|0,0,0)$

(7) $c \quad x,0,z$ $(m_y|0,0,\frac{1}{2})$

(8) $c \quad 0,y,z$ $(m_x|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
8	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	General: l : $l=2n$
							Special: no extra conditions
4	f	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	
4	e	. . 2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	
4	d	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	
4	c	2 . .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	
2	b	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			
2	a	. . 2/m	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $2mm$	Along [100] $\not{p}2mm$	Along [010] $\not{p}2mm$
	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}c2m$ ($\not{p}2cm$, 19)	1; 3; 6; 8
	[2] $\not{p}2cm$ (19)	1; 4; 6; 7
	[2] $\not{p}cc2$ (16)	1; 2; 7; 8
	[2] $\not{p}222$ (13)	1; 2; 3; 4
	[2] $\not{p}112/m$ (11)	1; 2; 5; 6
	[2] $\not{p}12/c1$ ($\not{p}2/c11$, 7)	1; 3; 5; 7
	[2] $\not{p}2/c11$ (7)	1; 4; 5; 8
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}ccm$ ($\mathbf{c}' = 3\mathbf{c}$) (21)

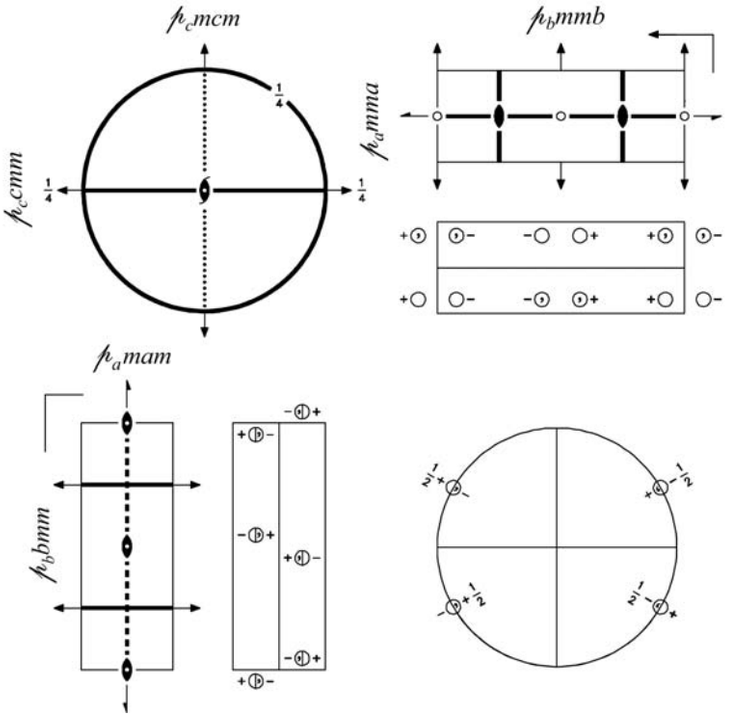
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{p}4/mcc$ (40); [2] $\not{p}4_2/mmc$ (41); [3] $\not{p}6/mcc$ (74)

II [2] $\not{p}mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (20)

$\not p mcm$ mmm Orthorhombic

No. 22 $\not p 2/m2/c2_1/m$ Patterson symmetry $\not p mmm$



Origin at centre $(2/m)$ at $2/mc2_1$

Asymmetric unit $0 \le x; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,y,\frac{1}{4}$ $(2_y|0,0,\frac{1}{2})$

(3) $2 \quad x,0,0$ $(2_x|0,0,0)$

(4) $2(\frac{1}{2}) \quad 0,0,z$ $(2_z|0,0,\frac{1}{2})$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $c \quad x,0,z$ $(m_y|0,0,\frac{1}{2})$

(7) $m \quad 0,y,z$ $(m_x|0,0,0)$

(8) $m \quad x,y,\frac{1}{4}$ $(m_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $x,\bar{y},\bar{z}$	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	no conditions
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,\bar{y},z+\frac{1}{2}$	(7) $\bar{x},y,z$	(8) $x,y,\bar{z}+\frac{1}{2}$	
							Special: no extra conditions
4	e	$..m$	$x,y,\frac{1}{4}$	$\bar{x},y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	
4	d	$m..$	$0,y,z$	$0,y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	$0,\bar{y},z+\frac{1}{2}$	
4	c	$2..$	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$\bar{x},0,0$	$x,0,\frac{1}{2}$	
2	b	$m2m$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			
2	a	$2/m..$	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $2mm$
Origin at $0,0,z$

Along [100] $\not{P}2mg$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $\not{P}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{P}2cm$ (19) 1; 3; 6; 8
[2] $\not{P}m2m$ ($\not{P}2mm$, 18) 1; 2; 7; 8
[2] $\not{P}mc2_1$ (17) 1; 4; 6; 7
[2] $\not{P}222_1$ (14) 1; 2; 3; 4
[2] $\not{P}112_1/m$ (12) 1; 4; 5; 8
[2] $\not{P}12/c1$ ($\not{P}2/c11$, 7) 1; 2; 5; 6
[2] $\not{P}2/m11$ (6) 1; 3; 5; 7

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{P}mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (22)

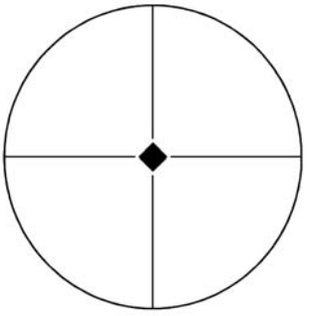
Minimal non-isotypic non-enantiomorphic supergroups

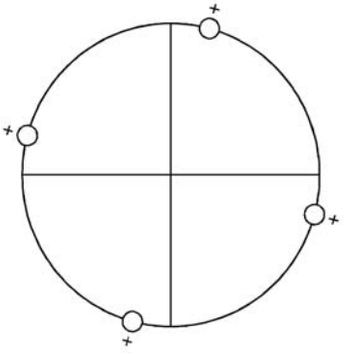
I [3] $\not{P}6_3/mmc$ (75)

II [2] $\not{P}mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (20)

$\not p4$ 4 Tetragonal

No. 23 $\not p4$ Patterson symmetry $\not p4/m$





Origin on 4

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
4 b 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$	no conditions
		Special: no extra conditions
1 a 4 . .	$0,0,z$	

Symmetry of special projections

Along [001] 4	Along [100] $\not{p}1\,1\,m$	Along [110] $\not{p}1\,1\,m$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,2$ (8) 1; 2

IIa none

IIb [2] $\not{p}4_2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}4$ ($\mathbf{c}' = 2\mathbf{c}$) (23)

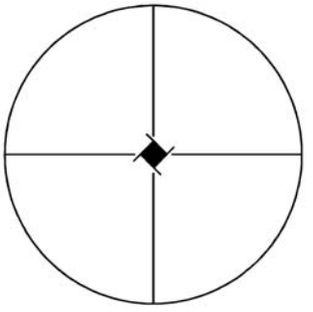
Minimal non-isotypic non-enantiomorphic supergroups

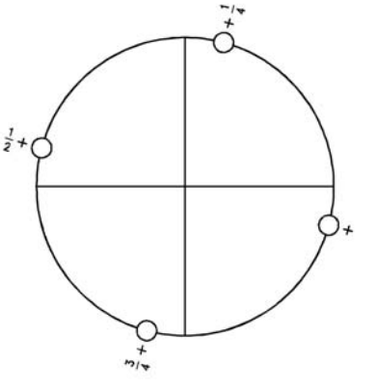
I [2] $\not{p}4/m$ (28); [2] $\not{p}4\,2\,2$ (30); [2] $\not{p}4\,m\,m$ (34); [2] $\not{p}4\,c\,c$ (36)

II none

$\not p 4_1$ 4 Tetragonal

No. 24 $\not p 4_1$ Patterson symmetry $\not p 4/m$





Origin on 4_1

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (1|0,0,0)

(2) $2(\frac{1}{2})$ 0,0,z (2_z|0,0,$\frac{1}{2}$)

(3) $4^+(\frac{1}{4})$ 0,0,z (4_z|0,0,$\frac{1}{4}$)

(4) $4^-(\frac{3}{4})$ 0,0,z (4_z^{-1}|0,0,$\frac{3}{4}$)

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	l : $l=4n$

Symmetry of special projections

Along [001] 4
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,2_1$ (9) 1; 2

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_3$ ($\mathbf{c}'=3\mathbf{c}$) (26); [5] $\not{p}4_1$ ($\mathbf{c}'=5\mathbf{c}$) (24)

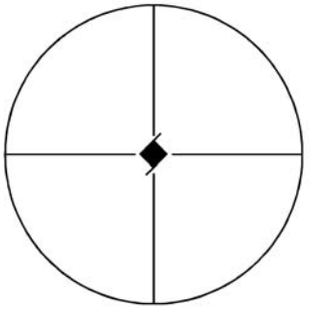
Minimal non-isotypic non-enantiomorphic supergroups

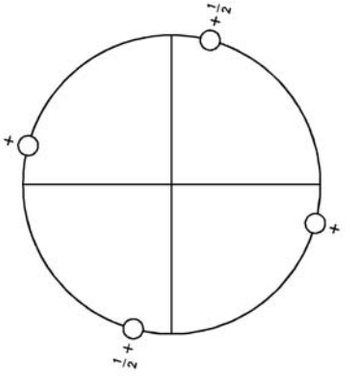
I [2] $\not{p}4_1\,2\,2$ (31)

II [2] $\not{p}4_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

$\not p 4_2$ 4 Tetragonal

No. 25 $\not p 4_2$ Patterson symmetry $\not p 4/m$





Origin on 2 on 4_2

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 2 0,0,z (2_z|0,0,0)

(3) $4^+(\frac{1}{2})$ 0,0,z (4_z|0,0,$\frac{1}{2}$)

(4) $4^-(\frac{1}{2})$ 0,0,z (4_z^{-1}|0,0,$\frac{1}{2}$)

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 *b* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	General: l : $l=2n$
2 *a* 2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			Special: no extra conditions

Symmetry of special projections

Along [001] 4	Along [100] $\not{p}1\,1\,m$	Along [110] $\not{p}1\,1\,m$
Origin at $0,0,z$	$\mathbf{a}'=\mathbf{c}$ Origin at $x,0,0$	$\mathbf{a}'=\mathbf{c}$ Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}1\,1\,2$ (8) 1; 2

IIa none

IIb [2] $\not{p}4_3$ ($\mathbf{c}'=2\mathbf{c}$) (26); [2] $\not{p}4_1$ ($\mathbf{c}'=2\mathbf{c}$) (24)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2$ ($\mathbf{c}'=3\mathbf{c}$) (25)

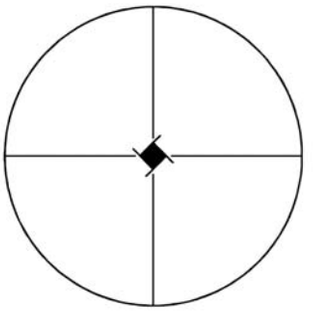
Minimal non-isotypic non-enantiomorphic supergroups

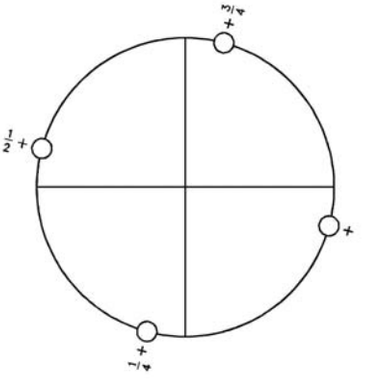
I [2] $\not{p}4_2/m$ (29); [2] $\not{p}4_2\,2\,2$ (32); [2] $\not{p}4_2\,c\,m$ (35)

II [2] $\not{p}4$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (23)

$\not p 4_3$ 4 Tetragonal

No. 26 $\not p 4_3$ Patterson symmetry $\not p 4/m$





Origin on 4_3

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(3) $4^+(\frac{3}{4})$ $0,0,z$ $(4_z|0,0,\frac{3}{4})$

(4) $4^-(\frac{1}{4})$ $0,0,z$ $(4_z^{-1}|0,0,\frac{1}{4})$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$	l : $l=4n$

Symmetry of special projections

Along [001] 4	Along [100] $\not{p}11g$	Along [110] $\not{p}11g$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}112_1$ (9) 1; 2

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_1$ ($\mathbf{c}'=3\mathbf{c}$) (24); [5] $\not{p}4_3$ ($\mathbf{c}'=5\mathbf{c}$) (26)

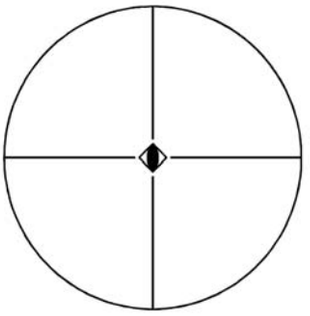
Minimal non-isotypic non-enantiomorphic supergroups

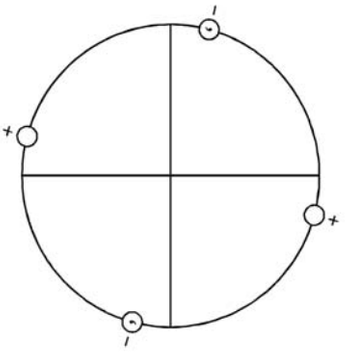
I [2] $\not{p}4_322$ (33)

II [2] $\not{p}4_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

$p\bar{4}$ $\bar{4}$ Tetragonal

No. 27 $p\bar{4}$ Patterson symmetry $p4/m$





Origin at $\bar{4}$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 2 $0,0,z$ $(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;\ 0,0,0$ $(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;\ 0,0,0$ $(\bar{4}_z^{-1}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	no conditions
							Special: no extra conditions
2	c	2 . .	$0,0,z$	$0,0,\bar{z}$			
1	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$				
1	a	$\bar{4}$ . .	$0,0,0$				

Symmetry of special projections

Along [001] 4
Origin at $0,0,z$

Along [100] $\not p 1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not p 1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not p 1\,1\,2$ (8) 1; 2

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not p\bar{4}$ ($\mathbf{c}' = 2\mathbf{c}$) (27)

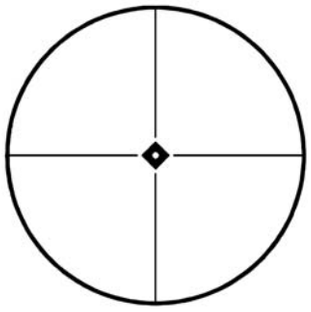
Minimal non-isotypic non-enantiomorphic supergroups

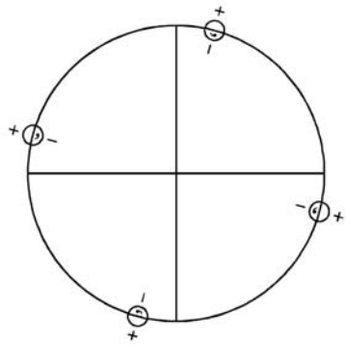
I [2] $\not p 4/m$ (28); [2] $\not p 4_2/m$ (29); [2] $\not p\bar{4}\,2\,m$ (37); [2] $\not p\bar{4}\,2\,c$ (38)

II none

$p4/m$ $4/m$ Tetragonal

No. 28 $p4/m$ Patterson symmetry $p4/m$





Origin at centre $(4/m)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \; 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \; 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$
$(m_z|0,0,0)$

(7) $\bar{4}^+ \; 0,0,z; \; 0,0,0$
$(\bar{4}_z|0,0,0)$

(8) $\bar{4}^- \; 0,0,z; \; 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	no conditions
							Special: no extra conditions
4	e	m . .	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	
4	d	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	
2	c	4 . .	$0,0,z$	$0,0,\bar{z}$			
1	b	$4/m$ . .	$0,0,\frac{1}{2}$				
1	a	$4/m$ . .	$0,0,0$				

Symmetry of special projections

Along [001] 4
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}\bar{4}$ (27) 1; 2; 7; 8
[2] $\not{p}4$ (23) 1; 2; 3; 4
[2] $\not{p}1\,1\,2/m$ (11) 1; 2; 5; 6

IIa none

IIb [2] $\not{p}4_2/m$ ($\mathbf{c}' = 2\mathbf{c}$) (29)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}4/m$ ($\mathbf{c}' = 2\mathbf{c}$) (28)

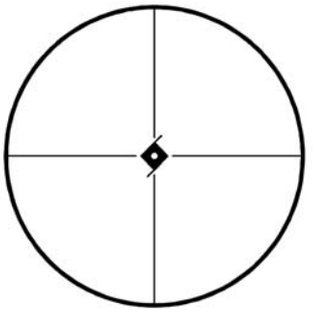
Minimal non-isotypic non-enantiomorphic supergroups

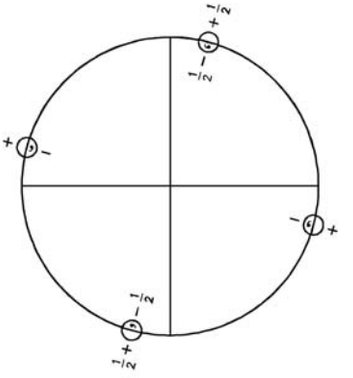
I [2] $\not{p}4/mmm$ (39); [2] $\not{p}4/mcc$ (40)

II none

$\not{p}4_2/m$ $4/m$ Tetragonal

No. 29 $\not{p}4_2/m$ Patterson symmetry $\not{p}4/m$





Origin at centre $(2/m)$ on 4_2

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+(\frac{1}{2}) \quad 0,0,z$
$(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2}) \quad 0,0,z$
$(4_z^{-1}|0,0,\frac{1}{2})$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$
$(m_z|0,0,0)$

(7) $\bar{4}^+ \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z|0,0,\frac{1}{2})$

(8) $\bar{4}^- \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z^{-1}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y,\bar{x},\bar{z}+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y},x,\bar{z}+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
4	d	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	
4	c	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	
2	b	$\bar{4}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			
2	a	$2/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] 4	Along [100] $\not{p}2mm$	Along [110] $\not{p}2mm$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}\bar{4}$ (27)	1; 2; 7; 8
	[2] $\not{p}4_2$ (25)	1; 2; 3; 4
	[2] $\not{p}1\,1\,2/m$ (11)	1; 2; 5; 6
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2/m$ ($\mathbf{c}'=3\mathbf{c}$) (29)

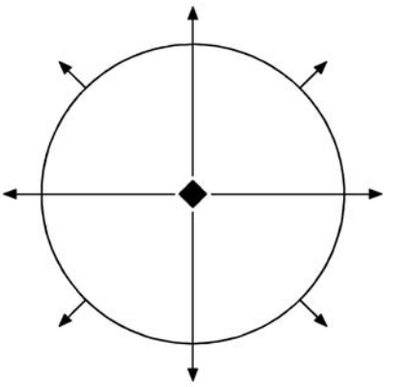
Minimal non-isotypic non-enantiomorphic supergroups

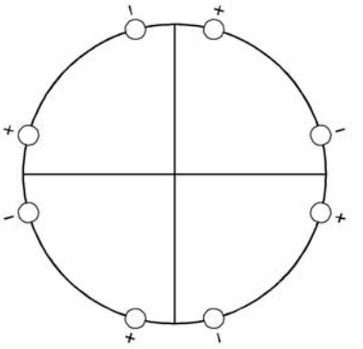
I [2] $\not{p}4_2/mmc$ (41)

II [2] $\not{p}4/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (28)

$p422$ 422 Tetragonal

No. 30 $p422$ Patterson symmetry $p4/mmm$





Origin at 422

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special: no extra conditions
4	g	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	
4	f	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	
4	e	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	
4	d	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	
2	c	4 . .	$0,0,z$	$0,0,\bar{z}$			
1	b	4 2 2	$0,0,\frac{1}{2}$				
1	a	4 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not P 2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not P 2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not P 4\,1\,1$ ($\not P 4$, 23) 1; 2; 3; 4
[2] $\not P 2\,2\,1$ ($\not P 2\,2\,2$, 13) 1; 2; 5; 6
[2] $\not P 2\,1\,2$ ($\not P 2\,2\,2$, 13) 1; 2; 7; 8

IIa none

IIb [2] $\not P 4_2\,2\,2$ ($\mathbf{c}' = 2\mathbf{c}$) (32)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not P 4\,2\,2$ ($\mathbf{c}' = 2\mathbf{c}$) (30)

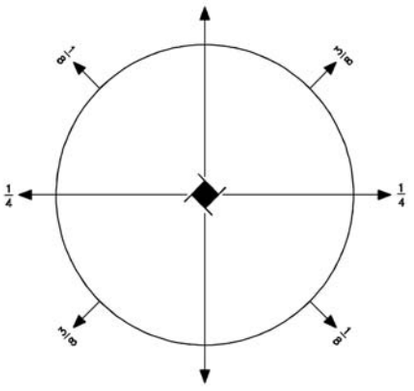
Minimal non-isotypic non-enantiomorphic supergroups

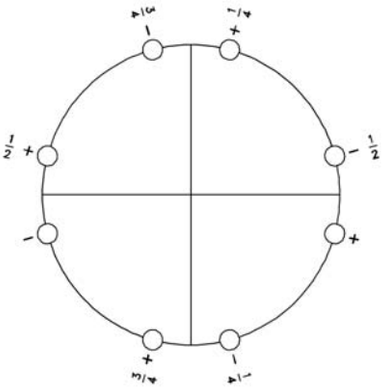
I [2] $\not P 4/mmm$ (39); [2] $\not P 4/mcc$ (40)

II none

$p4_122$ 422 Tetragonal

No. 31 $p4_122$ Patterson symmetry $p4/mmm$





Origin on $2[100]$ at $4_1(2,1)1$

Asymmetric unit $0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(3) $4^+(\frac{1}{4})$ $0,0,z$ $(4_z|0,0,\frac{1}{4})$

(4) $4^-(\frac{3}{4})$ $0,0,z$ $(4_z^{-1}|0,0,\frac{3}{4})$

(5) 2 $x,0,0$ $(2_x|0,0,0)$

(6) 2 $0,y,\frac{1}{4}$ $(2_y|0,0,\frac{1}{2})$

(7) 2 $x,x,\frac{1}{8}$ $(2_{xy}|0,0,\frac{1}{4})$

(8) 2 $x,\bar{x},\frac{3}{8}$ $(2_{\bar{x}y}|0,0,\frac{3}{4})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	l : $l=4n$
		(5) $x,\bar{y},\bar{z}$	(6) $\bar{x},y,\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{3}{4}$	
						Special: no extra conditions
4	b . . 2	$x,x,\frac{1}{8}$	$\bar{x},\bar{x},\frac{5}{8}$	$\bar{x},x,\frac{3}{8}$	$x,\bar{x},\frac{7}{8}$	
4	a . 2 .	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	

Symmetry of special projections

Along [001] $4mm$	Along [100] $\not{p}2mg$	Along [110] $\not{p}2mg$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,\frac{1}{8}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}4_1 11$ ($\not{p}4_1$, 24) 1; 2; 3; 4
[2] $\not{p}2_1 21$ ($\not{p}222_1$, 14) 1; 2; 5; 6
[2] $\not{p}2_1 12$ ($\not{p}222_1$, 14) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_3 22$ ($\mathbf{c}'=3\mathbf{c}$) (33); [5] $\not{p}4_1 22$ ($\mathbf{c}'=5\mathbf{c}$) (31)

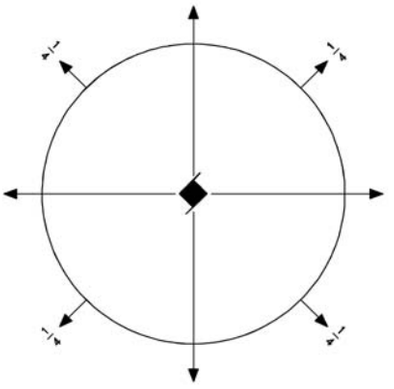
Minimal non-isotypic non-enantiomorphic supergroups

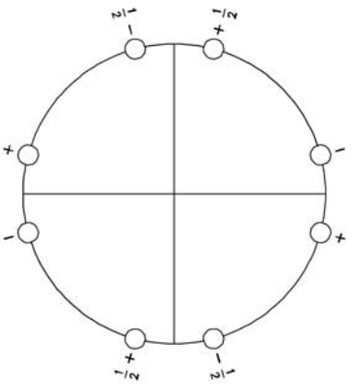
I none

II [2] $\not{p}4_2 22$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (32)

$\not p4_222$ 422 Tetragonal

No. 32 $\not p4_222$ Patterson symmetry $\not p4/mmm$





Origin at 222 at 4_221

Asymmetric unit $0 \le x; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $4^+(\frac{1}{2})$ $0,0,z$
$(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2})$ $0,0,z$
$(4_z^{-1}|0,0,\frac{1}{2})$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) 2 $x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) 2 $x,\bar{x},\frac{1}{4}$
$(2_{\bar{x}y}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
4	g	. . 2	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	
4	f	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	
4	e	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	
4	d	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	
4	c	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	
2	b	2 . 22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			
2	a	2 22 .	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}4_2 11$ ($\not{p}4_2$, 25) 1; 2; 3; 4
[2] $\not{p}2221$ ($\not{p}222$, 13) 1; 2; 5; 6
[2] $\not{p}2122$ ($\not{p}222$, 13) 1; 2; 7; 8

IIa none

IIb [2] $\not{p}4_3 22$ ($\mathbf{c}' = 2\mathbf{c}$) (33); [2] $\not{p}4_1 22$ ($\mathbf{c}' = 2\mathbf{c}$) (31)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2 22$ ($\mathbf{c}' = 3\mathbf{c}$) (32)

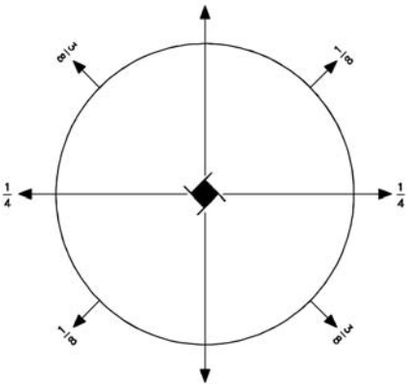
Minimal non-isotypic non-enantiomorphic supergroups

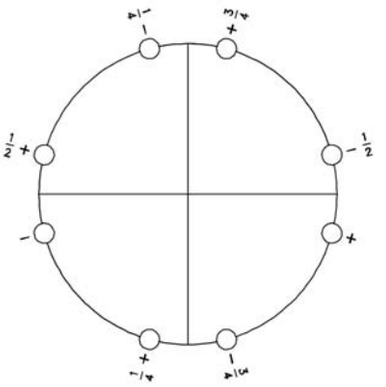
I [2] $\not{p}4_2/mmc$ (41)

II [2] $\not{p}422$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (30)

$\not p 4_3 22$ 422 Tetragonal

No. 33 $\not p 4_3 22$ Patterson symmetry $\not p 4/mmm$





Origin on $2[100]$ at $4_3(2,1)1$

Asymmetric unit $0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(3) $4^+(\frac{3}{4})$ $0,0,z$ $(4_z|0,0,\frac{3}{4})$

(4) $4^-(\frac{1}{4})$ $0,0,z$ $(4_z^{-1}|0,0,\frac{1}{4})$

(5) 2 $x,0,0$ $(2_x|0,0,0)$

(6) 2 $0,y,\frac{1}{4}$ $(2_y|0,0,\frac{1}{2})$

(7) 2 $x,x,\frac{3}{8}$ $(2_{xy}|0,0,\frac{3}{4})$

(8) 2 $x,\bar{x},\frac{1}{8}$ $(2_{\bar{x}y}|0,0,\frac{1}{4})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$	l : $l=4n$
		(5) $x,\bar{y},\bar{z}$	(6) $\bar{x},y,\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{3}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{4}$	
						Special: no extra conditions
4	b . . 2	$x,x,\frac{7}{8}$	$\bar{x},\bar{x},\frac{3}{8}$	$\bar{x},x,\frac{5}{8}$	$x,\bar{x},\frac{1}{8}$	
4	a . 2 .	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	

Symmetry of special projections

Along [001] $4mm$	Along [100] $\not{p}2mg$	Along [110] $\not{p}2mg$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,\frac{3}{8}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}4_3 11$ ($\not{p}4_3$, 26) 1; 2; 3; 4
[2] $\not{p}2_1 21$ ($\not{p}222_1$, 14) 1; 2; 5; 6
[2] $\not{p}2_1 12$ ($\not{p}222_1$, 14) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_1 22$ ($\mathbf{c}'=3\mathbf{c}$) (31); [5] $\not{p}4_3 22$ ($\mathbf{c}'=5\mathbf{c}$) (33)

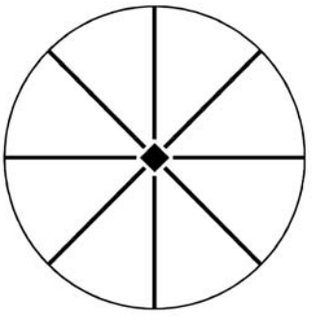
Minimal non-isotypic non-enantiomorphic supergroups

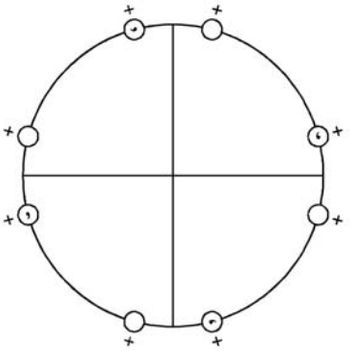
I none

II [2] $\not{p}4_2 22$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (32)

$p4mm$ $4mm$ Tetragonal

No. 34 $p4mm$ Patterson symmetry $p4/mmm$





Origin on $4mm$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \quad 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \quad 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $m \quad x,0,z$
$(m_y|0,0,0)$

(6) $m \quad 0,y,z$
$(m_x|0,0,0)$

(7) $m \quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) $m \quad x,x,z$
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special: no extra conditions
4	c	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	
4	b	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	
1	a	$4mm$	$0,0,z$				

Symmetry of special projections

Along [001] $4mm$	Along [100] $\not{p}11m$	Along [110] $\not{p}11m$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}411$ ($\not{p}4$, 23) 1; 2; 3; 4
[2] $\not{p}2m1$ ($\not{p}mm2$, 15) 1; 2; 5; 6
[2] $\not{p}21m$ ($\not{p}mm2$, 15) 1; 2; 7; 8

IIa none

IIb [2] $\not{p}4cc$ ($\mathbf{c}' = 2\mathbf{c}$) (36); [2] $\not{p}4_2mc$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}4_2cm$, 35); [2] $\not{p}4_2cm$ ($\mathbf{c}' = 2\mathbf{c}$) (35)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}4mm$ ($\mathbf{c}' = 2\mathbf{c}$) (34)

Minimal non-isotypic non-enantiomorphic supergroups

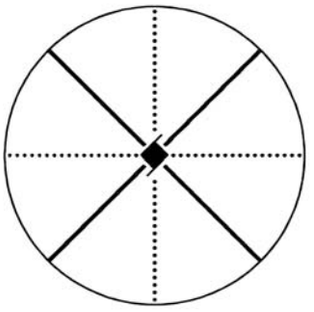
I [2] $\not{p}4/mmm$ (39)

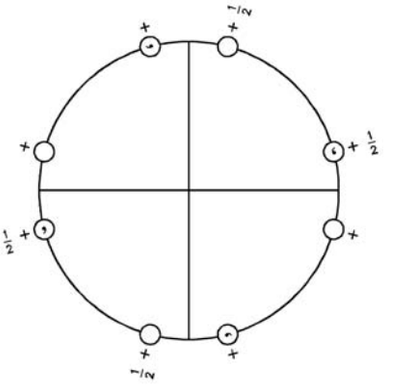
II none

$\not p 4_2 cm$ $4mm$ Tetragonal

No. 35 $\not p 4_2 cm$ Patterson symmetry $\not p 4/mmm$

FIRST SETTING





Origin on $2mm$ on 4_2cm

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,0,z$ $(2_z|0,0,0)$

(3) $4^+(\frac{1}{2}) \quad 0,0,z$ $(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2}) \quad 0,0,z$ $(4_z^{-1}|0,0,\frac{1}{2})$

(5) $c \quad x,0,z$ $(m_y|0,0,\frac{1}{2})$

(6) $c \quad 0,y,z$ $(m_x|0,0,\frac{1}{2})$

(7) $m \quad x,\bar{x},z$ $(m_{xy}|0,0,0)$

(8) $m \quad x,x,z$ $(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	l : $l=2n$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special: no extra conditions
4	b	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	
2	a	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}11m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}4_211$ ($\not{p}4_2$, 25) 1; 2; 3; 4
[2] $\not{p}2c1$ ($\not{p}cc2$, 16) 1; 2; 5; 6
[2] $\not{p}21m$ ($\not{p}mm2$, 15) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2cm$ ($\mathbf{c}'=3\mathbf{c}$) (35)

Minimal non-isotypic non-enantiomorphic supergroups

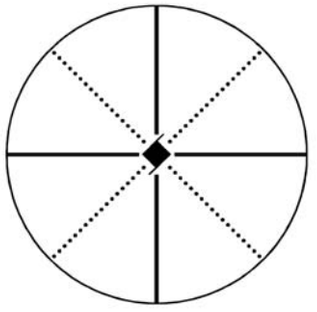
I [2] $\not{p}4_2/mmc$ (41)

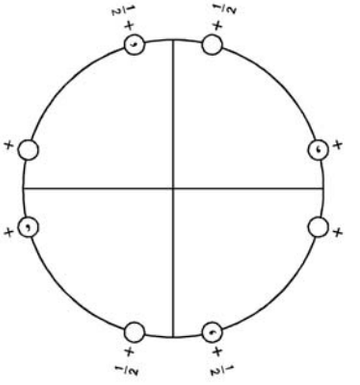
II [2] $\not{p}4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (34)

No. 35 $\not{p}4_2mc$

Patterson symmetry $\not{p}4/mmm$

SECOND SETTING





Origin on $2mm$ on 4_2mc

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $4^+(\frac{1}{2})$ $0,0,z$
$(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2})$ $0,0,z$
$(4_z^{-1}|0,0,\frac{1}{2})$

(5) m $x,0,z$
$(m_y|0,0,0)$

(6) m $0,y,z$
$(m_x|0,0,0)$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c x,x,z
$(m_{\bar{x}y}|0,0,\frac{1}{2})$

Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $y,x,z+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
4	b	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	
2	a	$2mm.$	$0,0,z$	$0,0,z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}4_211$ ($\not{p}4_2$, 25) 1; 2; 3; 4
[2] $\not{p}21c$ ($\not{p}cc2$, 16) 1; 2; 7; 8
[2] $\not{p}2m1$ ($\not{p}mm2$, 15) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2mc$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{p}4_2cm$, 35)

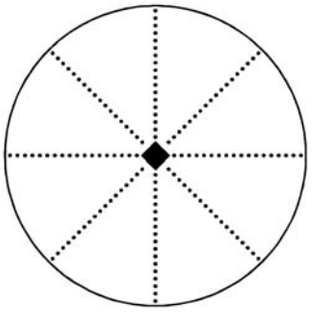
Minimal non-isotypic non-enantiomorphic supergroups

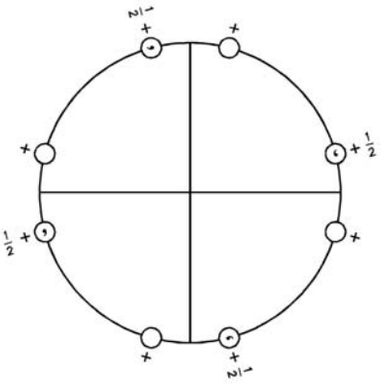
I [2] $\not{p}4_2/mmc$ (41)

II [2] $\not{p}4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (34)

$p4cc$ $4mm$ Tetragonal

No. 36 $p4cc$ Patterson symmetry $p4/mmm$





Origin on $4cc$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) c $x,0,z$
$(m_y|0,0,\frac{1}{2})$

(6) c $0,y,z$
$(m_x|0,0,\frac{1}{2})$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c x,x,z
$(m_{\bar{x}y}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	b 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	l : $l=2n$
		(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	
						Special: no extra conditions
2	a 4..	$0,0,z$	$0,0,z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}411$ ($\not{p}4$, 23) 1; 2; 3; 4
[2] $\not{p}2c1$ ($\not{p}cc2$, 16) 1; 2; 5; 6
[2] $\not{p}21c$ ($\not{p}cc2$, 16) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4cc$ ($\mathbf{c}'=3\mathbf{c}$) (36)

Minimal non-isotypic non-enantiomorphic supergroups

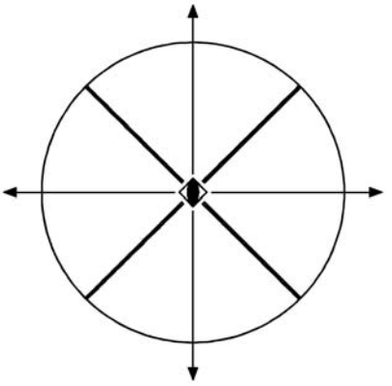
I [2] $\not{p}4/mcc$ (40)

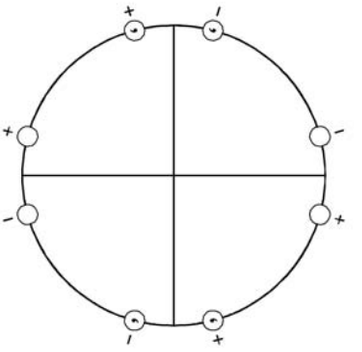
II [2] $\not{p}4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (34)

$p\bar{4}2m$ $\bar{4}2m$ Tetragonal

No. 37 $p\bar{4}2m$ Patterson symmetry $p4/mmm$

FIRST SETTING





Origin at $\bar{4}2m$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z$; $0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m x,x,z
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	no conditions
							Special: no extra conditions
4	f	. . m	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	
4	e	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	
4	d	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	
2	c	2 . mm	$0,0,z$	$0,0,\bar{z}$			
1	b	$\bar{4}$ 2 m	$0,0,\frac{1}{2}$				
1	a	$\bar{4}$ 2 m	$0,0,0$				

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}11m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}\bar{4}11$ ($\not{p}\bar{4}$, 27) 1; 2; 3; 4
[2] $\not{p}21m$ ($\not{p}mm2$, 15) 1; 2; 7; 8
[2] $\not{p}221$ ($\not{p}222$, 13) 1; 2; 5; 6

IIa none

IIb [2] $\not{p}\bar{4}2c$ ($\mathbf{c}' = 2\mathbf{c}$) (38)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{4}2m$ ($\mathbf{c}' = 2\mathbf{c}$) (37)

Minimal non-isotypic non-enantiomorphic supergroups

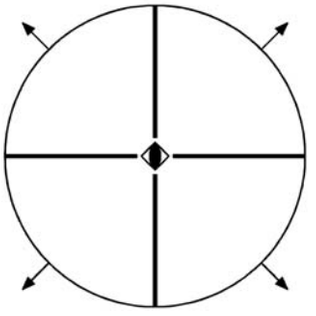
I [2] $\not{p}4/mmm$ (39); [2] $\not{p}4_2/mmc$ (41)

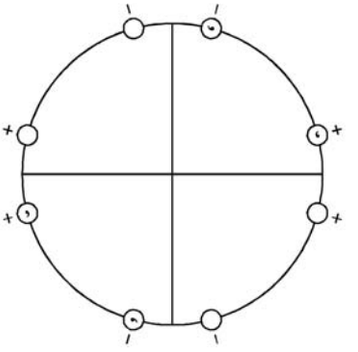
II none

No. 37 $p\bar{4}m2$

Patterson symmetry $p4/mmm$

SECOND SETTING





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;\ 0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;\ 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) m $x,0,z$
$(m_y|0,0,0)$

(6) m $0,y,z$
$(m_x|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special: no extra conditions
4	f	. m .	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$	
4	e	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	
4	d	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$	
2	c	2 mm .	$0,0,z$	$0,0,\bar{z}$			
1	b	$\bar{4}$ m 2	$0,0,\frac{1}{2}$				
1	a	$\bar{4}$ m 2	$0,0,0$				

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}\bar{4}\,1\,1$ ($\not{p}\bar{4}$, 27) 1; 2; 3; 4
[2] $\not{p}2\,m\,1$ ($\not{p}mm2$, 15) 1; 2; 5; 6
[2] $\not{p}2\,1\,2$ ($\not{p}222$, 13) 1; 2; 7; 8

IIa none

IIb [2] $\not{p}\bar{4}\,c\,2$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{4}\,2\,c$, 38)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{4}\,m\,2$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{4}\,2\,m$, 37)

Minimal non-isotypic non-enantiomorphic supergroups

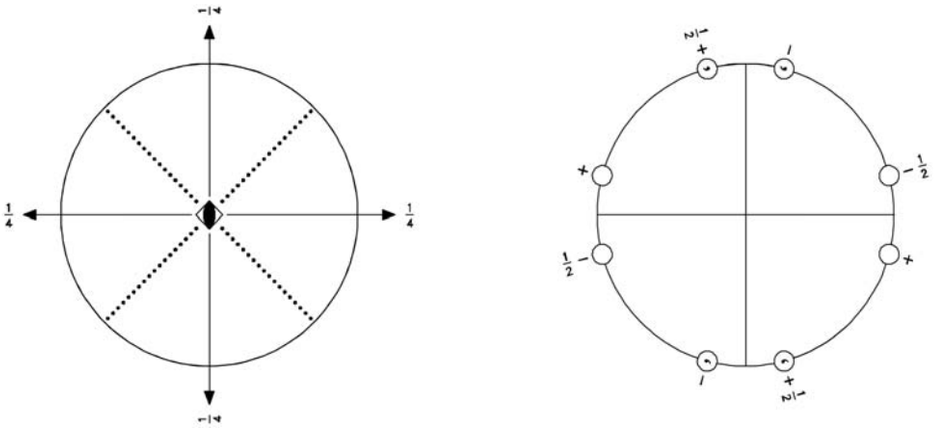
I [2] $\not{p}4/mmm$ (39); [2] $\not{p}4_2/mmc$ (41)

II none

$p\bar{4}2c$ $\bar{4}2m$ Tetragonal

No. 38 $p\bar{4}2c$ Patterson symmetry $p4/mmm$

FIRST SETTING



Origin at $\bar{4}1c$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;\ 0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;\ 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) 2 $0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(6) 2 $x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c x,x,z
$(m_{\bar{x}y}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $y,x,z+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,z+\frac{1}{2}$	
4	d	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$y,0,\frac{3}{4}$	$\bar{y},0,\frac{3}{4}$	
4	c	. 2 .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	
2	b	$\bar{4}$ . .	$0,0,0$	$0,0,\frac{1}{2}$			
2	a	2 22 .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 27) 1; 2; 3; 4
[2] $p21c$ ($pcc2$, 16) 1; 2; 7; 8
[2] $p221$ ($p222$, 13) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $p\bar{4}2c$ ($\mathbf{c}' = 3\mathbf{c}$) (38)

Minimal non-isotypic non-enantiomorphic supergroups

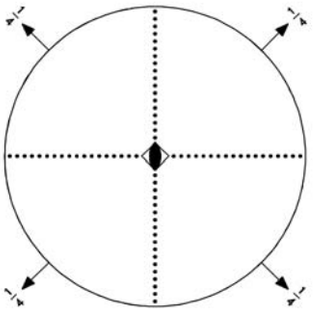
I [2] $p4/mcc$ (40); [2] $p4_2/mmc$ (41)

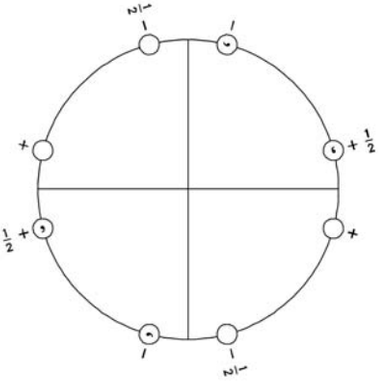
II [2] $p\bar{4}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (37)

No. 38 $\not{p}\bar{4}c2$

Patterson symmetry $\not{p}4/mmm$

SECOND SETTING





Origin at $\bar{4}c1$

Asymmetric unit $0 \le x; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;\ 0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;\ 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) c $x,0,z$
$(m_y|0,0,\frac{1}{2})$

(6) c $0,y,z$
$(m_x|0,0,\frac{1}{2})$

(7) 2 $x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) 2 $x,\bar{x},\frac{1}{4}$
$(2_{\bar{x}y}|0,0,\frac{1}{2})$

Generators selected (1); $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	l : $l=2n$
							Special: no extra conditions
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	
4	d	. . 2	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	
4	c	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
2	b	$\bar{4}$ . .	$0,0,0$	$0,0,\frac{1}{2}$			
2	a	2 . 22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 27) 1; 2; 3; 4
[2] $P2c1$ ($Pcc2$, 16) 1; 2; 5; 6
[2] $P212$ ($P222$, 13) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P\bar{4}c2$ ($\mathbf{c}' = 3\mathbf{c}$) ($P\bar{4}2c$, 38)

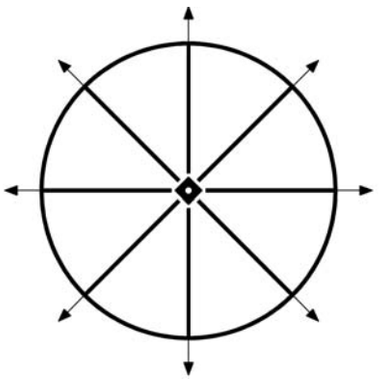
Minimal non-isotypic non-enantiomorphic supergroups

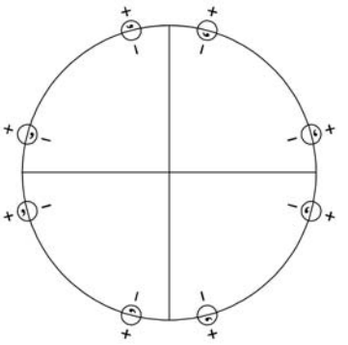
I [2] $P4/mcc$ (40); [2] $P4_2/mmc$ (41)

II [2] $P\bar{4}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (37)

$p4/mmm$ $4/mmm$ Tetragonal

No. 39 $p4/m2/m2/m$ Patterson symmetry $p4/mmm$





Origin at centre $(4/mmm)$

Asymmetric unit $0 \le x;\quad 0 \le y;\quad 0 \le z \le \frac{1}{2};\quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2\quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+\ 0,0,z$
$(4_z|0,0,0)$

(4) $4^-\ 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2\quad 0,y,0$
$(2_y|0,0,0)$

(6) $2\quad x,0,0$
$(2_x|0,0,0)$

(7) $2\quad x,x,0$
$(2_{xy}|0,0,0)$

(8) $2\quad x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

(9) $\bar{1}\quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $m\quad x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+\ 0,0,z;\ 0,0,0$
$(\bar{4}_z|0,0,0)$

(12) $\bar{4}^-\ 0,0,z;\ 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(13) $m\quad x,0,z$
$(m_y|0,0,0)$

(14) $m\quad 0,y,z$
$(m_x|0,0,0)$

(15) $m\quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(16) $m\quad x,x,z$
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: no extra conditions
8	k	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	
			$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	$0,x,\bar{z}$	$0,\bar{x},\bar{z}$	
8	j	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	
			$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	i	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	h	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,0$	$\bar{y},\bar{x},0$	
4	g	$m\,2m.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	
4	f	$m\,2m.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	
4	e	$m.2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	
4	d	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	
2	c	$4\,m\,m$	$0,0,z$	$0,0,\bar{z}$			
1	b	$4/m\,m\,m$	$0,0,\frac{1}{2}$				
1	a	$4/m\,m\,m$	$0,0,0$				

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{2}mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{2}mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{4}\bar{4}2m$ (37)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $\not{4}\bar{4}m2$ ($\not{4}\bar{4}2m$, 37)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $\not{4}4mm$ (34)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $\not{4}422$ (30)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $\not{4}4/m11$ ($\not{4}4/m$, 28)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $\not{2}2/m2/m1$ ($\not{4}mmm$, 20)	1; 2; 5; 6; 9; 10; 13; 14
	[2] $\not{2}2/m12/m$ ($\not{4}mmm$, 20)	1; 2; 7; 8; 9; 10; 15; 16
IIa	none	
IIb	[2] $\not{4}4_2/mmc$ ($\mathbf{c}' = 2\mathbf{c}$) (41); [2] $\not{4}4_2/mcm$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{4}4_2/mmc$, 41); [2] $\not{4}4/mcc$ ($\mathbf{c}' = 2\mathbf{c}$) (40)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{4}4/mmm$ ($\mathbf{c}' = 2\mathbf{c}$) (39)

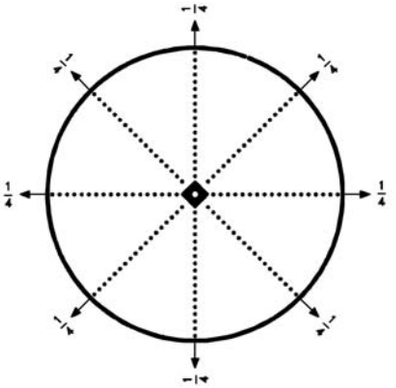
Minimal non-isotypic non-enantiomorphic supergroups

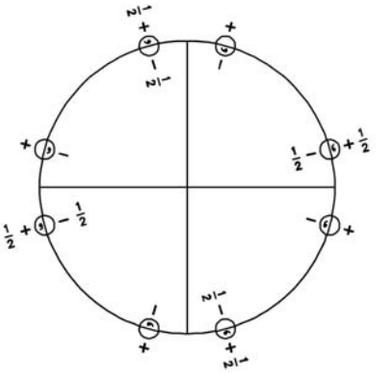
I none

II none

$\not{p}4/mcc$ $4/mmm$ Tetragonal

No. 40 $\not{p}4/m2/c2/c$ Patterson symmetry $\not{p}4/mmm$





Origin at centre $(4/m)$ at $4/mcc$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \quad 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \quad 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2 \quad 0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(6) $2 \quad x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(7) $2 \quad x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) $2 \quad x,\bar{x},\frac{1}{4}$
$(2_{\bar{x}y}|0,0,\frac{1}{2})$

(9) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $m \quad x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z|0,0,0)$

(12) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(13) $c \quad x,0,z$
$(m_y|0,0,\frac{1}{2})$

(14) $c \quad 0,y,z$
$(m_x|0,0,\frac{1}{2})$

(15) $c \quad x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(16) $c \quad x,x,z$
$(m_{\bar{x}y}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	l : $l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	
							Special: no extra conditions
8	f	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	e	. 2 .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$0,\bar{x},\frac{1}{4}$	
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	
8	d	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	
			$\bar{x},\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
4	c	4 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	
2	b	$4/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$			
2	a	4 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}\bar{4}2c$ (38)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $\not{p}\bar{4}c2$ ($\not{p}\bar{4}2c$, 38)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $\not{p}4cc$ (36)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $\not{p}422$ (30)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $\not{p}4/m11$ ($\not{p}4/m$, 28)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $\not{p}2/m2/c1$ ($\not{p}ccm$, 21)	1; 2; 5; 6; 9; 10; 13; 14
	[2] $\not{p}2/m12/c$ ($\not{p}ccm$, 21)	1; 2; 7; 8; 9; 10; 15; 16
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4/mcc$ ($\mathbf{c}' = 3\mathbf{c}$) (40)

Minimal non-isotypic non-enantiomorphic supergroups

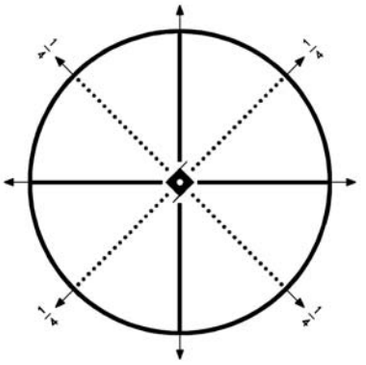
I none

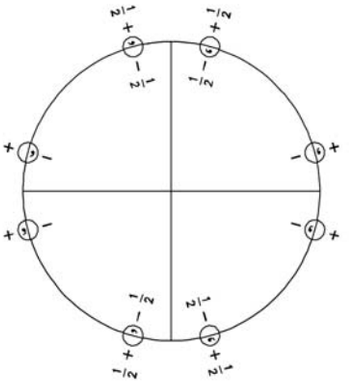
II [2] $\not{p}4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (39)

$\not{p}4_2/mmc$ $4/mmm$ Tetragonal

No. 41 $\not{p}4_2/m2/m2/c$ Patterson symmetry $\not{p}4/mmm$

FIRST SETTING





Origin at centre (mmm) at $4_2/m2/mc$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+(\frac{1}{2}) \quad 0,0,z$
$(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2}) \quad 0,0,z$
$(4_z^{-1}|0,0,\frac{1}{2})$

(5) $2 \quad 0,y,0$
$(2_y|0,0,0)$

(6) $2 \quad x,0,0$
$(2_x|0,0,0)$

(7) $2 \quad x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) $2 \quad x,\bar{x},\frac{1}{4}$
$(2_{\bar{x}y}|0,0,\frac{1}{2})$

(9) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $m \quad x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z|0,0,\frac{1}{2})$

(12) $\bar{4}^- \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z^{-1}|0,0,\frac{1}{2})$

(13) $m \quad x,0,z$
$(m_y|0,0,0)$

(14) $m \quad 0,y,z$
$(m_x|0,0,0)$

(15) $c \quad x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(16) $c \quad x,x,z$
$(m_{\bar{x}y}|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	l : $l=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	
							Special: no extra conditions
8	h	. m .	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z+\frac{1}{2}$	$y,0,z+\frac{1}{2}$	
			$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$y,0,\bar{z}+\frac{1}{2}$	$\bar{y},0,\bar{z}+\frac{1}{2}$	
8	g	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	f	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	
			$\bar{x},\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	
4	e	m 2m .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	
4	d	m 2m .	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	
4	c	2 mm .	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	
2	b	$\bar{4}$ m 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			
2	a	m mm .	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $P\bar{4}2c$ (38)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P\bar{4}m2$ ($P\bar{4}2m$, 37)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P4_2mc$ ($P4_2cm$, 35)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (32)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 29)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Pccm$, 21)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/m1$ ($Pmmm$, 20)	1; 2; 5; 6; 9; 10; 13; 14
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P4_2/mmc$ ($\mathbf{c}' = 3\mathbf{c}$) (41)

Minimal non-isotypic non-enantiomorphic supergroups

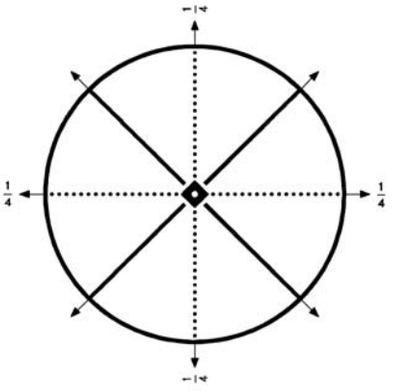
I none

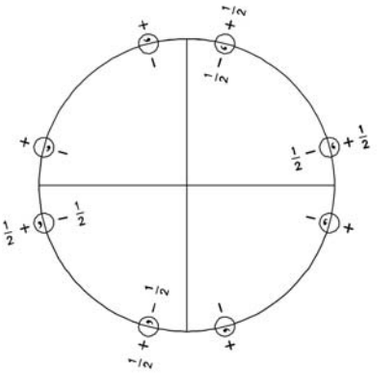
II [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (39)

No. 41 $P4_2/m2/c2/m$

Patterson symmetry $P4/mmm$

SECOND SETTING





Origin at centre (mmm) at $4_2/mc2/m$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+(\frac{1}{2}) \quad 0,0,z$
$(4_z|0,0,\frac{1}{2})$

(4) $4^-(\frac{1}{2}) \quad 0,0,z$
$(4_z^{-1}|0,0,\frac{1}{2})$

(5) $2 \quad 0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(6) $2 \quad x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(7) $2 \quad x,x,0$
$(2_{xy}|0,0,0)$

(8) $2 \quad x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

(9) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $m \quad x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z|0,0,\frac{1}{2})$

(12) $\bar{4}^- \quad 0,0,z; \quad 0,0,\frac{1}{4}$
$(\bar{4}_z^{-1}|0,0,\frac{1}{2})$

(13) $c \quad x,0,z$
$(m_y|0,0,\frac{1}{2})$

(14) $c \quad 0,y,z$
$(m_x|0,0,\frac{1}{2})$

(15) $m \quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(16) $m \quad x,x,z$
$(m_{\bar{x}y}|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$l\ :\ l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: no extra conditions
8	h	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	
			$\bar{x},x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	g	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$	
8	f	$.2.$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	$0,x,\frac{1}{4}$	
4	e	$m.2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,0$	$x,\bar{x},0$	
4	d	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	
4	c	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	
2	b	$\bar{4}2m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			
2	a	$m.mm$	$0,0,0$	$0,0,\frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}\bar{4}c2$ ($\not{p}\bar{4}2c$, 38)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $\not{p}\bar{4}2m$ (37)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $\not{p}4_2cm$ (35)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $\not{p}4_222$ (32)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $\not{p}4_2/m11$ ($\not{p}4_2/m$, 29)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $\not{p}2/m2/c1$ ($\not{p}ccm$, 21)	1; 2; 5; 6; 9; 10; 13; 14
	[2] $\not{p}2/m12/m$ ($\not{p}mmm$, 20)	1; 2; 7; 8; 9; 10; 15; 16
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}4_2/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) ($\not{p}4_2/mmc$, 41)

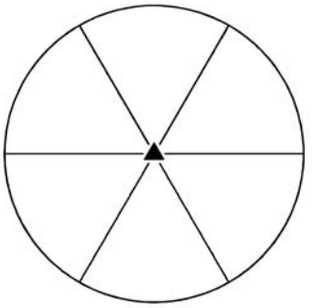
Minimal non-isotypic non-enantiomorphic supergroups

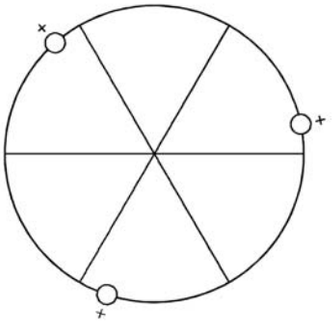
I none

II [2] $\not{p}4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (39)

$p\bar{3}$ 3 Trigonal

No. 42 $p\bar{3}$ Patterson symmetry $p\bar{3}$





Origin on 3

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 3^+ 0,0,z (3_z|0,0,0)

(3) 3^- 0,0,z (3_z^{-1}|0,0,0)

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
3 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$		no conditions
					Special: no extra conditions
1 a 3 . .	$0,0,z$				

Symmetry of special projections

Along [001] 3	Along [100] $P\bar{1}$	Along [210] $P\bar{1}$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I [3] $P\bar{1}$ (1) 1

IIa none

IIb [3] $P\bar{3}_2$ ($\mathbf{c}' = 3\mathbf{c}$) (44); [3] $P\bar{3}_1$ ($\mathbf{c}' = 3\mathbf{c}$) (43)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $P\bar{3}$ ($\mathbf{c}' = 2\mathbf{c}$) (42)

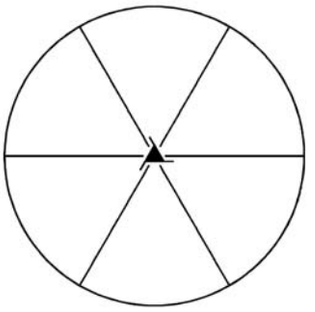
Minimal non-isotypic non-enantiomorphic supergroups

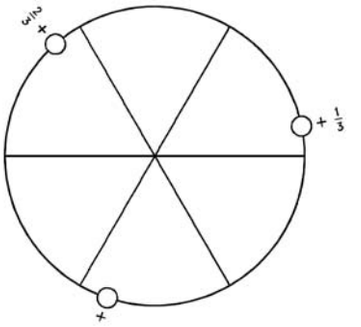
I [2] $P\bar{3}$ (45); [2] $P\bar{3}\,1\,2$ (46); [2] $P\bar{3}\,m\,1$ (49); [2] $P\bar{3}\,c\,1$ (50); [2] $P\bar{6}$ (53); [2] $P\bar{6}_3$ (56); [2] $P\bar{6}$ (59)

II none

$\not p 3_1$ 3 Trigonal

No. 43 $\not p 3_1$ Patterson symmetry $\not p \bar{3}$





Origin on 3_1

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$ $(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{2}{3})$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
3 a 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{1}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	l : $l=3n$

Symmetry of special projections

Along [001] 3	Along [100] $\not{P}1$	Along [210] $\not{P}1$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [3] $\not{P}1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{P}3_2$ ($\mathbf{c}'=2\mathbf{c}$) (44); [7] $\not{P}3_1$ ($\mathbf{c}'=7\mathbf{c}$) (43)

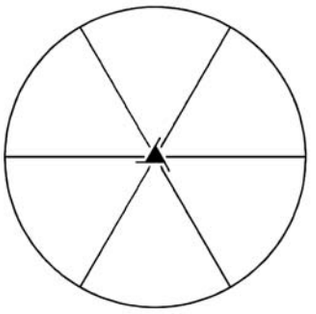
Minimal non-isotypic non-enantiomorphic supergroups

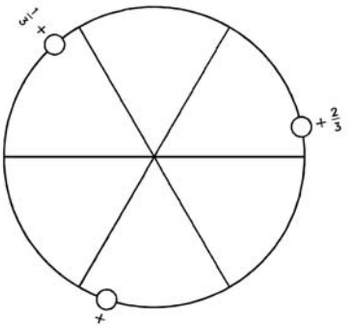
I [2] $\not{P}3_1 12$ (47); [2] $\not{P}6_1$ (54); [2] $\not{P}6_4$ (57)

II [3] $\not{P}3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (42)

$\not p 3_2$ 3 Trigonal

No. 44 $\not p 3_2$ Patterson symmetry $\not p \bar{3}$





Origin on 3_2

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$ $(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{1}{3})$

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Generators selected (1); $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
3 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	l : $l=3n$

Symmetry of special projections

Along [001] 3
Origin at $0,0,z$

Along [100] $P1$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $P1$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [3] $P1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

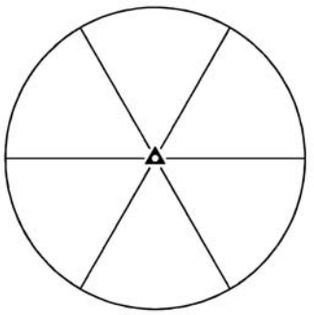
IIc [2] $P3_1$ ($\mathbf{c}'=2\mathbf{c}$) (43); [7] $P3_2$ ($\mathbf{c}'=7\mathbf{c}$) (44)

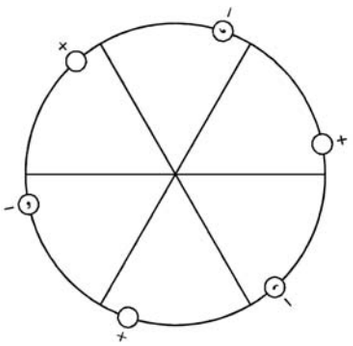
Minimal non-isotypic non-enantiomorphic supergroups

I [2] $P3_2 12$ (48); [2] $P6_2$ (55); [2] $P6_5$ (58)
II [3] $P3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (42)

$p\bar{3}$ $\bar{3}$ Trigonal

No. 45 $p\bar{3}$ Patterson symmetry $p\bar{3}$





Origin at centre ($\bar{3}$)

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(5) $\bar{3}^+$ $0,0,z$; $0,0,0$
$(\bar{3}_z|0,0,0)$

(6) $\bar{3}^-$ $0,0,z$; $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $y,\bar{x}+y,\bar{z}$	(6) $x-y,x,\bar{z}$	
						Special: no extra conditions
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	$\bar{3}$ . .	$0,0,\frac{1}{2}$			
1	a	$\bar{3}$ . .	$0,0,0$			

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{p}2\,1\,1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}2\,1\,1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3$ (42) 1; 2; 3
[3] $\not{p}\bar{1}$ (2) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{3}$ ($\mathbf{c}' = 2\mathbf{c}$) (45)

Minimal non-isotypic non-enantiomorphic supergroups

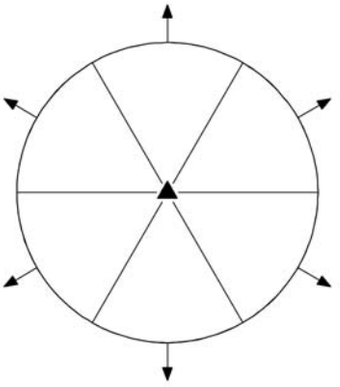
I [2] $\not{p}\bar{3}\,1\,m$ (51); [2] $\not{p}\bar{3}\,1\,c$ (52); [2] $\not{p}6/m$ (60); [2] $\not{p}6_3/m$ (61)

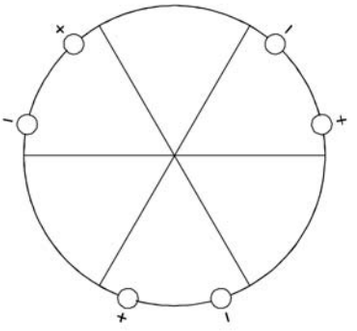
II none

$p312$ 312 Trigonal

No. 46 $p312$ Patterson symmetry $p\bar{3}1m$

FIRST SETTING





Origin at 312

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(5) 2 $x,2x,0$
$(2_2|0,0,0)$

(6) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$	
						Special: no extra conditions
3	e	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	d	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	3 . 2	$0,0,\frac{1}{2}$			
1	a	3 . 2	$0,0,0$			

Symmetry of special projections

Along [001] $3m$	Along [100] $\not{p}1m1$	Along [210] $\not{p}211$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}311$ ($\not{p}3$, 42) 1; 2; 3
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 4
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 5
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 6

IIa none

IIb [3] $\not{p}3_{2}12$ ($\mathbf{c}'=3\mathbf{c}$) (48); [3] $\not{p}3_{1}12$ ($\mathbf{c}'=3\mathbf{c}$) (47)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}312$ ($\mathbf{c}'=2\mathbf{c}$) (46)

Minimal non-isotypic non-enantiomorphic supergroups

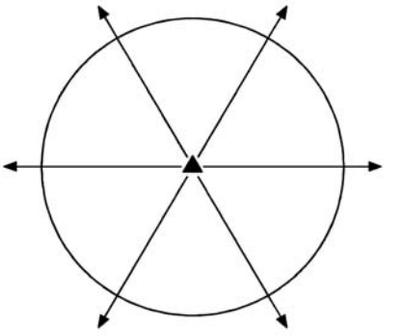
I [2] $\not{p}\bar{3}1m$ (51); [2] $\not{p}\bar{3}1c$ (52); [2] $\not{p}622$ (62); [2] $\not{p}6_{3}22$ (65); [2] $\not{p}\bar{6}m2$ (71); [2] $\not{p}\bar{6}c2$ (72)

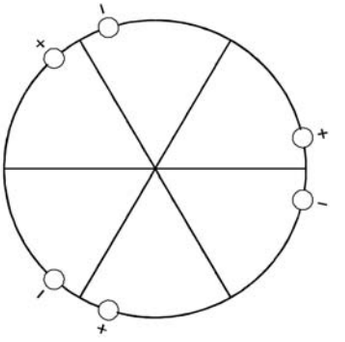
II none

No. 46 $p321$

Patterson symmetry $p\bar{3}m1$

SECOND SETTING





Origin at 321

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(5) 2 $x,0,0$
$(2_x|0,0,0)$

(6) 2 $0,y,0$
$(2_y|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$	no conditions
						Special: no extra conditions
3	e	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	d	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	3 2 .	$0,0,\frac{1}{2}$			
1	a	3 2 .	$0,0,0$			

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $\not{P}211$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{P}1m1$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{P}311$ ($\not{P}3$, 42) 1; 2; 3
[3] $\not{P}121$ ($\not{P}211$, 3) 1; 4
[3] $\not{P}121$ ($\not{P}211$, 3) 1; 5
[3] $\not{P}121$ ($\not{P}211$, 3) 1; 6

IIa none

IIb [3] $\not{P}3_{2}21$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{P}3_{2}12$, 48); [3] $\not{P}3_{1}21$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{P}3_{1}12$, 47)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{P}321$ ($\mathbf{c}'=2\mathbf{c}$) ($\not{P}312$, 46)

Minimal non-isotypic non-enantiomorphic supergroups

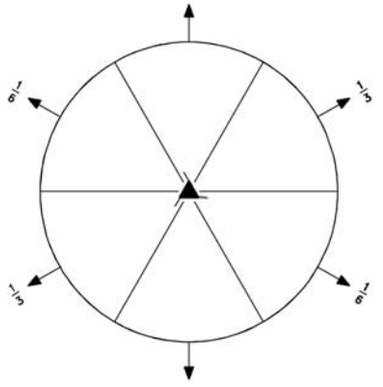
I [2] $\not{P}\bar{3}1m$ (51); [2] $\not{P}\bar{3}1c$ (52); [2] $\not{P}622$ (62); [2] $\not{P}6_{3}22$ (65); [2] $\not{P}\bar{6}m2$ (71); [2] $\not{P}\bar{6}c2$ (72)

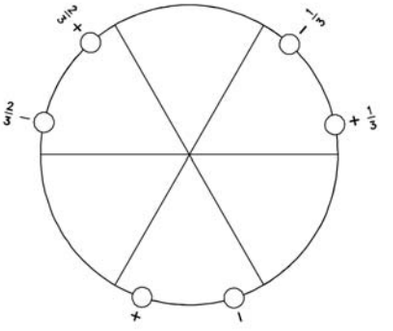
II none

$\not p 3_1 1 2$ 312 Trigonal

No. 47 $\not p 3_1 1 2$ Patterson symmetry $\not p \bar{3} 1 m$

FIRST SETTING





Origin on $2[210]$ at $3_1 1(1,1,2)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$ $(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{2}{3})$

(4) 2 $x,\bar{x},\frac{1}{3}$ $(2_3|0,0,\frac{2}{3})$

(5) 2 $x,2x,\frac{1}{6}$ $(2_2|0,0,\frac{1}{3})$

(6) 2 $2x,x,0$ $(2_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6	c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	General:
		(4) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{1}{3}$	(6) $x,x-y,\bar{z}$	l : $l=3n$
					Special: no extra conditions
3	b . . 2	$x,\bar{x},\frac{5}{6}$	$x,2x,\frac{1}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	a . . 2	$x,\bar{x},\frac{1}{3}$	$x,2x,\frac{2}{3}$	$2\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $3m$	Along [100] $\not{p}1m1$	Along [210] $\not{p}211$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{1}{6}$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3_1 11$ ($\not{p}3_1$, 43) 1; 2; 3
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 4
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 5
[3] $\not{p}112$ ($\not{p}211$, 3) 1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}3_2 12$ ($\mathbf{c}'=2\mathbf{c}$) (48); [7] $\not{p}3_1 12$ ($\mathbf{c}'=7\mathbf{c}$) (47)

Minimal non-isotypic non-enantiomorphic supergroups

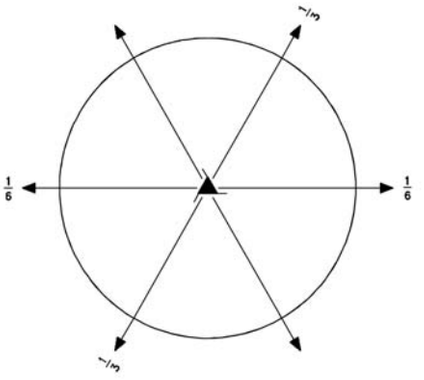
I [2] $\not{p}6_1 22$ (63); [2] $\not{p}6_4 22$ (66)

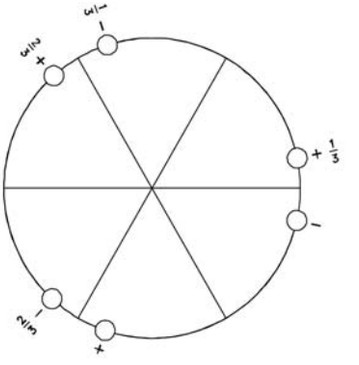
II [3] $\not{p}312$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (46)

No. 47 $\not{p}3_121$

Patterson symmetry $\not{p}\bar{3}m1$

SECOND SETTING





Origin on $2[110]$ at $3_1(1,1,2)1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$ $(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{2}{3})$

(4) 2 $x,x,0$ $(2_{xy}|0,0,0)$

(5) 2 $x,0,\frac{1}{3}$ $(2_x|0,0,\frac{2}{3})$

(6) 2 $0,y,\frac{1}{6}$ $(2_y|0,0,\frac{1}{3})$

Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6	c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	General:
		(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{2}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	l : $l=3n$
					Special: no extra conditions
3	b . 2 .	$x,0,\frac{5}{6}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a . 2 .	$x,0,\frac{1}{3}$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $P2\,1\,1$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,\frac{1}{3}$

Along [210] $P1\,m\,1$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{6}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P3_1\,1\,1$ ($P3_1$, 43) 1; 2; 3
[3] $P1\,2\,1$ ($P2\,1\,1$, 3) 1; 4
[3] $P1\,2\,1$ ($P2\,1\,1$, 3) 1; 5
[3] $P1\,2\,1$ ($P2\,1\,1$, 3) 1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $P3_2\,2\,1$ ($\mathbf{c}'=2\mathbf{c}$) ($P3_2\,1\,2$, 48); [7] $P3_1\,2\,1$ ($\mathbf{c}'=7\mathbf{c}$) ($P3_1\,1\,2$, 47)

Minimal non-isotypic non-enantiomorphic supergroups

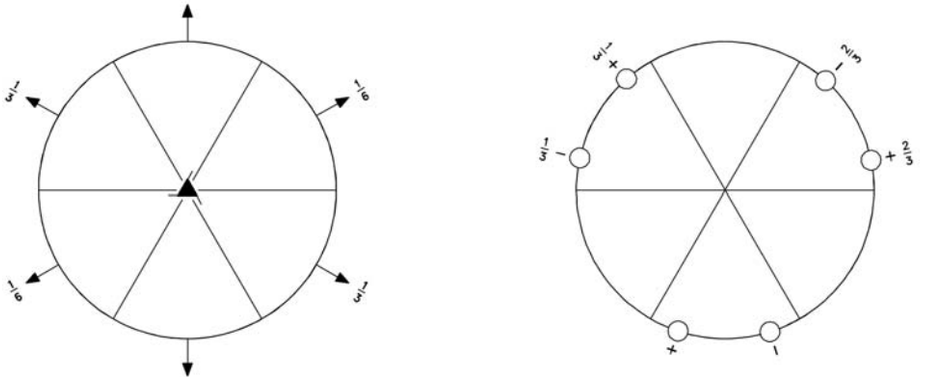
I [2] $P6_1\,2\,2$ (63); [2] $P6_4\,2\,2$ (66)

II [3] $P3\,1\,2$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (46)

$\not p 3_2 12$ 312 Trigonal

No. 48 $\not p 3_2 12$ Patterson symmetry $\not p \bar{3} 1m$

FIRST SETTING



Origin on $2[210]$ at $3_2 1(1,1,2)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$ $(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{1}{3})$

(4) 2 $x,\bar{x},\frac{1}{6}$ $(2_3|0,0,\frac{1}{3})$

(5) 2 $x,2x,\frac{1}{3}$ $(2_2|0,0,\frac{2}{3})$

(6) 2 $2x,x,0$ $(2_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$		l : $l=3n$
	(4) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{2}{3}$	(6) $x,x-y,\bar{z}$		
					Special: no extra conditions
3 b . . 2	$x,\bar{x},\frac{1}{6}$	$x,2x,\frac{5}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$		
3 a . . 2	$x,\bar{x},\frac{2}{3}$	$x,2x,\frac{1}{3}$	$2\bar{x},\bar{x},0$		

Symmetry of special projections

Along [001] $3m$	Along [100] $P1m1$	Along [210] $P211$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{1}{3}$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $P3_2 11$ ($P3_2$, 44)	1; 2; 3
	[3] $P112$ ($P211$, 3)	1; 4
	[3] $P112$ ($P211$, 3)	1; 5
	[3] $P112$ ($P211$, 3)	1; 6
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $P3_1 12$ ($\mathbf{c}'=2\mathbf{c}$) (47); [7] $P3_2 12$ ($\mathbf{c}'=7\mathbf{c}$) (48)

Minimal non-isotypic non-enantiomorphic supergroups

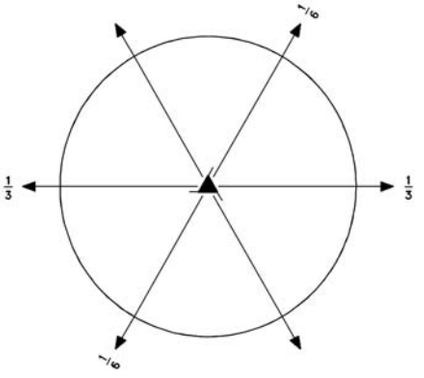
I [2] $P6_2 22$ (64); [2] $P6_5 22$ (67)

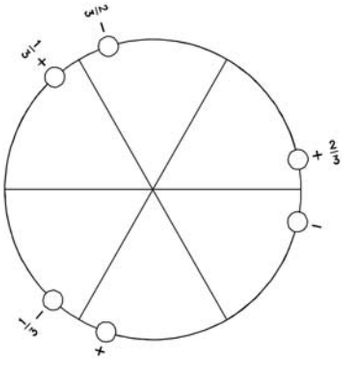
II [3] $P312$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (46)

No. 48 $\not{p}3_221$

Patterson symmetry $\not{p}\bar{3}m1$

SECOND SETTING





Origin on $2[110]$ at $3_2(1,1,2)1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$
$(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{1}{3})$

(4) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(5) 2 $x,0,\frac{1}{6}$
$(2_x|0,0,\frac{1}{3})$

(6) 2 $0,y,\frac{1}{3}$
$(2_y|0,0,\frac{2}{3})$

Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 c 1		(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$l \;:\; l=3n$
		(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	
					Special: no extra conditions
3 b . 2 .		$x,0,\frac{1}{6}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3 a . 2 .		$x,0,\frac{2}{3}$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $3m$	Along [100] $P\bar{2}11$	Along [210] $P\bar{1}m1$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{1}{6}$	Origin at $x,\frac{1}{2}x,\frac{1}{3}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P\bar{3}_2 11$ ($P\bar{3}_2$, 44) 1; 2; 3
[3] $P\bar{1}21$ ($P\bar{2}11$, 3) 1; 4
[3] $P\bar{1}21$ ($P\bar{2}11$, 3) 1; 5
[3] $P\bar{1}21$ ($P\bar{2}11$, 3) 1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $P\bar{3}_1 21$ ($\mathbf{c}'=2\mathbf{c}$) ($P\bar{3}_1 12$, 47); [7] $P\bar{3}_2 21$ ($\mathbf{c}'=7\mathbf{c}$) ($P\bar{3}_2 12$, 48)

Minimal non-isotypic non-enantiomorphic supergroups

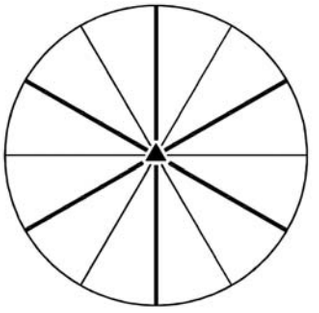
I [2] $P\bar{6}_2 22$ (64); [2] $P\bar{6}_5 22$ (67)

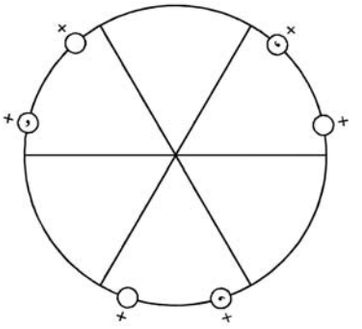
II [3] $P\bar{3}12$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (46)

$\not p 3m1$ $3m1$ Trigonal

No. 49 $\not p 3m1$ Patterson symmetry $\not p \bar{3} m1$

FIRST SETTING





Origin on $3m1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad x \le 2y; \quad y \le 2x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(5) m $x,2x,z$
$(m_x|0,0,0)$

(6) m $2x,x,z$
$(m_y|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$	
						Special: no extra conditions
3	b	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
1	a	$3m.$	$0,0,z$			

Symmetry of special projections

Along [001] $3m$	Along [100] $\not{p}1$	Along [210] $\not{p}11m$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}31\,1$ ($\not{p}3$, 42)	1; 2; 3
	[3] $\not{p}1\,m\,1$ ($\not{p}m\,11$, 4)	1; 4
	[3] $\not{p}1\,m\,1$ ($\not{p}m\,11$, 4)	1; 5
	[3] $\not{p}1\,m\,1$ ($\not{p}m\,11$, 4)	1; 6
IIa	none	
IIb	[2] $\not{p}3\,c\,1$ ($\mathbf{c}' = 2\mathbf{c}$) (50)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}3\,m\,1$ ($\mathbf{c}' = 2\mathbf{c}$) (49)

Minimal non-isotypic non-enantiomorphic supergroups

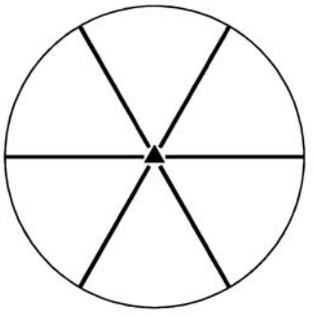
I [2] $\not{p}\bar{3}\,1\,m$ (51); [2] $\not{p}6\,m\,m$ (68); [2] $\not{p}6_3\,m\,c$ (70); [2] $\not{p}\bar{6}\,m\,2$ (71)

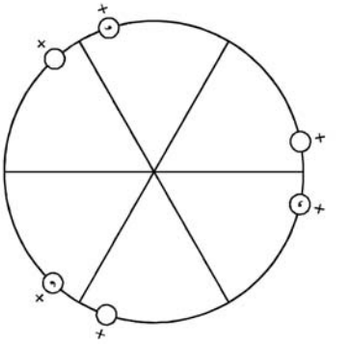
II none

No. 49 $\not{p}31m$

Patterson symmetry $\not{p}\bar{3}1m$

SECOND SETTING





Origin on 31m

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m x,x,z
$(m_3|0,0,0)$

(5) m $x,0,z$
$(m_2|0,0,0)$

(6) m $0,y,z$
$(m_1|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 c 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$		no conditions
	(4) y,x,z	(5) $x-y,\bar{y},z$	(6) $\bar{x},\bar{x}+y,z$		
					Special: no extra conditions
3 b . . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$		
1 a 3 . m	$0,0,z$				

Symmetry of special projections

Along [001] $3m$	Along [100] $\not{p}11m$	Along [210] $\not{p}1$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}311$ ($\not{p}3$, 42)	1; 2; 3
	[3] $\not{p}11m$ ($\not{p}m11$, 4)	1; 4
	[3] $\not{p}11m$ ($\not{p}m11$, 4)	1; 5
	[3] $\not{p}11m$ ($\not{p}m11$, 4)	1; 6
IIa	none	
IIb	[2] $\not{p}31c$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}3c1$, 50)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}31m$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}3m1$, 49)

Minimal non-isotypic non-enantiomorphic supergroups

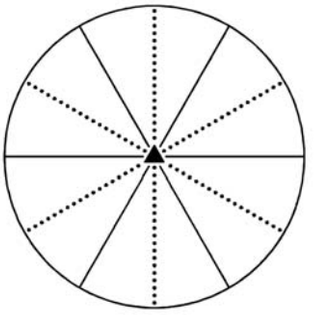
I [2] $\not{p}\bar{3}1m$ (51); [2] $\not{p}6mm$ (68); [2] $\not{p}6_3mc$ (70); [2] $\not{p}\bar{6}m2$ (71)

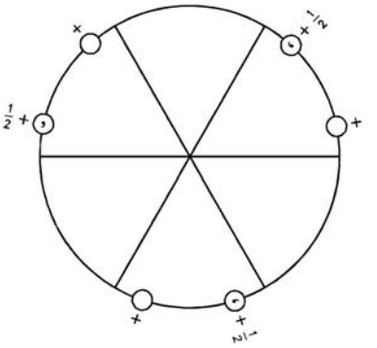
II none

$\not p 3\,c\,1$ $3\,m\,1$ Trigonal

No. 50 $\not p 3\,c\,1$ Patterson symmetry $\not p \bar{3}\,m\,1$

FIRST SETTING





Origin on $3c1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 3^+ $0,0,z$ $(3_z|0,0,0)$

(3) 3^- $0,0,z$ $(3_z^{-1}|0,0,0)$

(4) c $x,\bar{x},z$ $(m_{xy}|0,0,\frac{1}{2})$

(5) c $x,2x,z$ $(m_x|0,0,\frac{1}{2})$

(6) c $2x,x,z$ $(m_y|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$		l : $l=2n$
	(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$		
					Special: no extra conditions
2 a 3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $\not{p}1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3\,1\,1$ ($\not{p}3$, 42) 1; 2; 3
[3] $\not{p}1\,c\,1$ ($\not{p}c\,1\,1$, 5) 1; 4
[3] $\not{p}1\,c\,1$ ($\not{p}c\,1\,1$, 5) 1; 5
[3] $\not{p}1\,c\,1$ ($\not{p}c\,1\,1$, 5) 1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}3\,c\,1$ ($\mathbf{c}'=3\mathbf{c}$) (50)

Minimal non-isotypic non-enantiomorphic supergroups

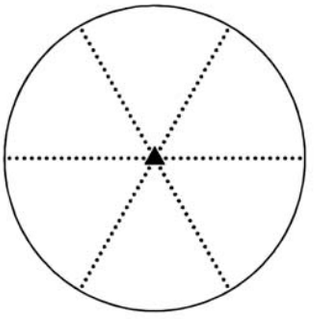
I [2] $\not{p}\bar{3}\,1\,c$ (52); [2] $\not{p}6\,c\,c$ (69); [2] $\not{p}6_3\,m\,c$ (70); [2] $\not{p}\bar{6}\,c\,2$ (72)

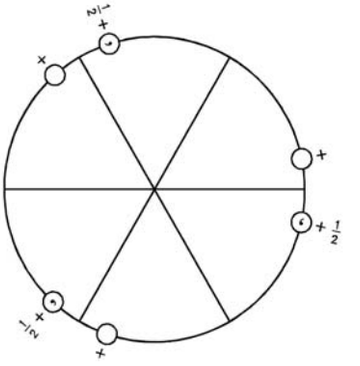
II [2] $\not{p}3\,m\,1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (49)

No. 50 $\not{p}31c$

Patterson symmetry $\not{p}\bar{3}1m$

SECOND SETTING





Origin on 31c

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 3^+ $0,0,z$ $(3_z|0,0,0)$

(3) 3^- $0,0,z$ $(3_z^{-1}|0,0,0)$

(4) c x,x,z $(m_3|0,0,\frac{1}{2})$

(5) c $x,0,z$ $(m_2|0,0,\frac{1}{2})$

(6) c $0,y,z$ $(m_1|0,0,\frac{1}{2})$

Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
	(4) $y,x,z+\frac{1}{2}$	(5) $x-y,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	
				Special: no extra conditions
2 a 3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$		

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3\,1\,1$ ($\not{p}3$, 42) 1; 2; 3
[3] $\not{p}1\,1\,c$ ($\not{p}c\,1\,1$, 5) 1; 4
[3] $\not{p}1\,1\,c$ ($\not{p}c\,1\,1$, 5) 1; 5
[3] $\not{p}1\,1\,c$ ($\not{p}c\,1\,1$, 5) 1; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}3\,1\,c$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{p}3\,c\,1$, 50)

Minimal non-isotypic non-enantiomorphic supergroups

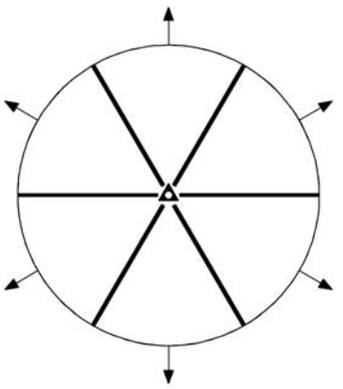
I [2] $\not{p}\bar{3}\,1\,c$ (52); [2] $\not{p}6\,c\,c$ (69); [2] $\not{p}6_3\,m\,c$ (70); [2] $\not{p}\bar{6}\,c\,2$ (72)

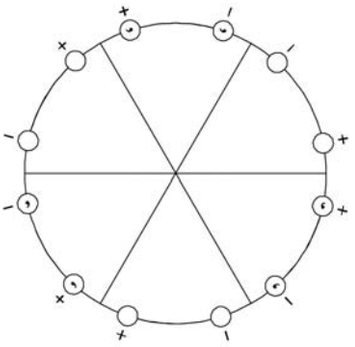
II [2] $\not{p}3\,m\,1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (49)

$p\bar{3}1m$ $\bar{3}1m$ Trigonal

No. 51 $p\bar{3}12/m$ Patterson symmetry $p\bar{3}1m$

FIRST SETTING





Origin at centre $(\bar{3}1m)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(5) 2 $x,2x,0$
$(2_2|0,0,0)$

(6) 2 $2x,x,0$
$(2_1|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
12	g	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) y,x,z	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x},\bar{x}+y,z$	General: no conditions
						Special: no extra conditions
6	f	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$
6	e	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$
6	d	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$
2	c	3 . m	$0,0,z$	$0,0,\bar{z}$				
1	b	$\bar{3}$. m	$0,0,\frac{1}{2}$					
1	a	$\bar{3}$. m	$0,0,0$					

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{P}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{P}211$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{P}31m$ ($\not{P}3m1$, 49)	1; 2; 3; 10; 11; 12
	[2] $\not{P}312$ (46)	1; 2; 3; 4; 5; 6
	[2] $\not{P}\bar{3}11$ ($\not{P}\bar{3}$, 45)	1; 2; 3; 7; 8; 9
	[3] $\not{P}112/m$ ($\not{P}2/m11$, 6)	1; 4; 7; 10
	[3] $\not{P}112/m$ ($\not{P}2/m11$, 6)	1; 5; 7; 11
	[3] $\not{P}112/m$ ($\not{P}2/m11$, 6)	1; 6; 7; 12
IIa	none	
IIb	[2] $\not{P}\bar{3}1c$ ($\mathbf{c}' = 2\mathbf{c}$) (52)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{P}\bar{3}1m$ ($\mathbf{c}' = 2\mathbf{c}$) (51)

Minimal non-isotypic non-enantiomorphic supergroups

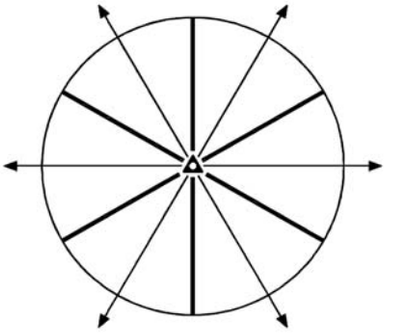
I [2] $\not{P}6/mmm$ (73); [2] $\not{P}6_3/mmc$ (75)

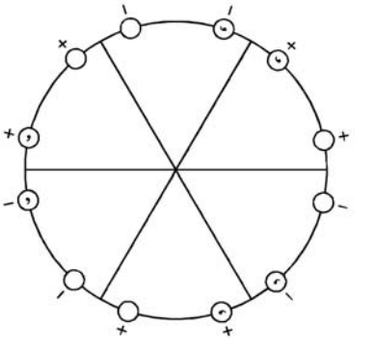
II none

No. 51 $\not{p}\bar{3}2/m1$

Patterson symmetry $\not{p}\bar{3}m1$

SECOND SETTING





Origin at centre $(\bar{3}m1)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x/2$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(5) 2 $x,0,0$
$(2_x|0,0,0)$

(6) 2 $0,y,0$
$(2_y|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(11) m $x,2x,z$
$(m_x|0,0,0)$

(12) m $2x,x,z$
$(m_y|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$				
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$				
									Special: no extra conditions
6	f	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	
6	e	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	d	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
2	c	3 m .	$0,0,z$	$0,0,\bar{z}$					
1	b	$\bar{3}$ m .	$0,0,\frac{1}{2}$						
1	a	$\bar{3}$ m .	$0,0,0$						

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}211$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3m1$ (49) 1; 2; 3; 10; 11; 12
[2] $\not{p}321$ ($\not{p}312$, 46) 1; 2; 3; 4; 5; 6
[2] $\not{p}\bar{3}11$ ($\not{p}\bar{3}$, 45) 1; 2; 3; 7; 8; 9
[3] $\not{p}12/m1$ ($\not{p}2/m11$, 6) 1; 4; 7; 10
[3] $\not{p}12/m1$ ($\not{p}2/m11$, 6) 1; 5; 7; 11
[3] $\not{p}12/m1$ ($\not{p}2/m11$, 6) 1; 6; 7; 12

IIa none

IIb [2] $\not{p}\bar{3}c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{3}1c$, 52)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{3}m1$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{3}1m$, 51)

Minimal non-isotypic non-enantiomorphic supergroups

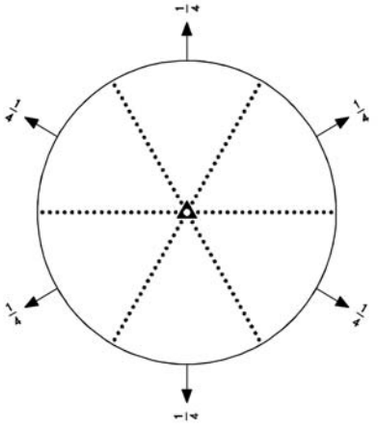
I [2] $\not{p}6/mmm$ (73); [2] $\not{p}6_3/mmc$ (75)

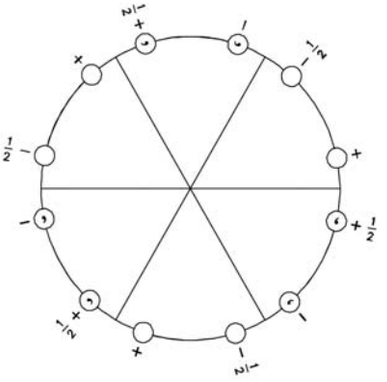
II none

$\not{p}\bar{3}1c$ $\bar{3}1m$ Trigonal

No. 52 $\not{p}\bar{3}12/c$ Patterson symmetry $\not{p}\bar{3}1m$

FIRST SETTING





Origin at centre $(\bar{3})$ at $\bar{3}1c$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,\bar{x},\frac{1}{4}$
$(2_3|0,0,\frac{1}{2})$

(5) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(6) 2 $2x,x,\frac{1}{4}$
$(2_1|0,0,\frac{1}{2})$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(11) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(12) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	e	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $y,x,z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $x-y,\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	l : $l=2n$
						Special: no extra conditions
6	d	. . 2	$x,\bar{x},\frac{1}{4}$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$
4	c	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$		
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$				
2	a	3 . 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}211$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}31c$ ($\not{p}3c1$, 50) 1; 2; 3; 10; 11; 12
[2] $\not{p}312$ (46) 1; 2; 3; 4; 5; 6
[2] $\not{p}\bar{3}11$ ($\not{p}\bar{3}$, 45) 1; 2; 3; 7; 8; 9
[3] $\not{p}112/c$ ($\not{p}2/c11$, 7) 1; 4; 7; 10
[3] $\not{p}112/c$ ($\not{p}2/c11$, 7) 1; 5; 7; 11
[3] $\not{p}112/c$ ($\not{p}2/c11$, 7) 1; 6; 7; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}\bar{3}1c$ ($\mathbf{c}'=3\mathbf{c}$) (52)

Minimal non-isotypic non-enantiomorphic supergroups

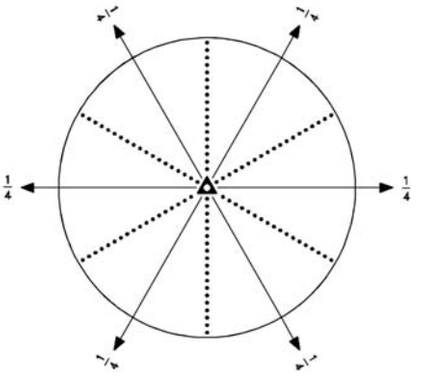
I [2] $\not{p}6/mcc$ (74); [2] $\not{p}6_3/mmc$ (75)

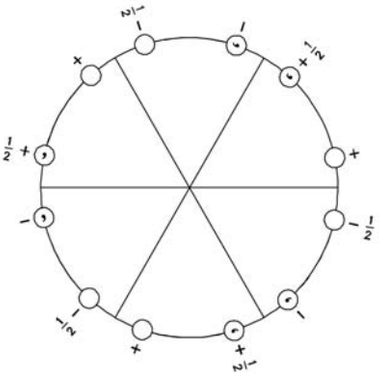
II [2] $\not{p}\bar{3}1m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (51)

No. 52 $\not{p}\bar{3}2/c1$

Patterson symmetry $\not{p}\bar{3}m1$

SECOND SETTING





Origin at centre $(\bar{3})$ at $\bar{3}c1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(5) 2 $x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(6) 2 $0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(11) c $x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(12) c $2x,x,z$
$(m_y|0,0,\frac{1}{2})$

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	e	1	(1) x,y,z (4) $y,x,\bar{z}+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $\bar{y},\bar{x},z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{x}+y,y,z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $x,x-y,z+\frac{1}{2}$	l : $l=2n$
						Special: no extra conditions
6	d	. 2 .	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$
4	c	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$		
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$				
2	a	3 2 .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				

Symmetry of special projections

Along [001] $6mm$	Along [100] $p2\,1\,1$	Along [210] $p2mg$
	$\mathbf{a}'=\frac{1}{2}\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $P3c1$ (50)	1; 2; 3; 10; 11; 12
	[2] $P321$ ($P312$, 46)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 45)	1; 2; 3; 7; 8; 9
	[3] $P12/c1$ ($P2/c11$, 7)	1; 4; 7; 10
	[3] $P12/c1$ ($P2/c11$, 7)	1; 5; 7; 11
	[3] $P12/c1$ ($P2/c11$, 7)	1; 6; 7; 12
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P\bar{3}c1$ ($\mathbf{c}'=3\mathbf{c}$) ($P\bar{3}1c$, 52)

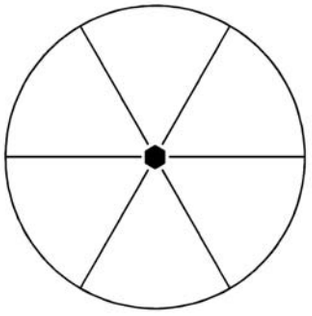
Minimal non-isotypic non-enantiomorphic supergroups

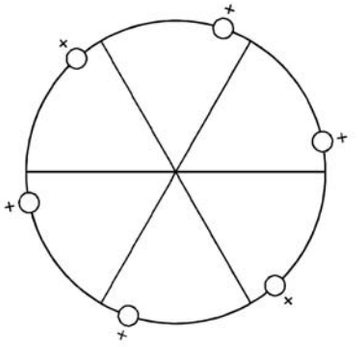
I [2] $P6/mcc$ (74); [2] $P6_3/mmc$ (75)

II [2] $P\bar{3}1m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (51)

$\not p6$ 6 Hexagonal

No. 53 $\not p6$ Patterson symmetry $\not p6/m$





Origin on 6

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$		no conditions
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$		
					Special: no extra conditions
1 a 6	$0,0,z$				

Symmetry of special projections

Along [001] 6	Along [100] $\not{p}1\,1\,m$	Along [210] $\not{p}1\,1\,m$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3$ (42) 1; 2; 3
[3] $\not{p}1\,1\,2$ (8) 1; 4

IIa none

IIb [2] $\not{p}6_3$ ($\mathbf{c}' = 2\mathbf{c}$) (56); [3] $\not{p}6_4$ ($\mathbf{c}' = 3\mathbf{c}$) (57); [3] $\not{p}6_2$ ($\mathbf{c}' = 3\mathbf{c}$) (55)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}6$ ($\mathbf{c}' = 2\mathbf{c}$) (53)

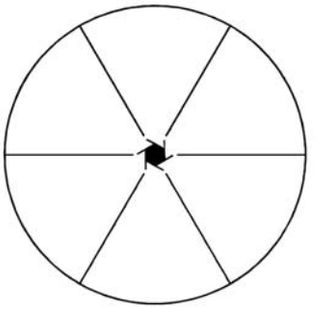
Minimal non-isotypic non-enantiomorphic supergroups

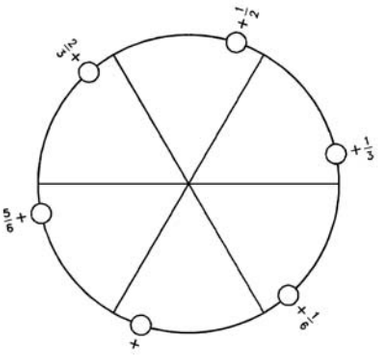
I [2] $\not{p}6/m$ (60); [2] $\not{p}6\,2\,2$ (62); [2] $\not{p}6mm$ (68); [2] $\not{p}6cc$ (69)

II none

$\not p 6_1$ 6 Hexagonal

No. 54 $\not p 6_1$ Patterson symmetry $\not p 6/m$





Origin on 6_1

Asymmetric unit $0 \le z \le \frac{1}{6}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$ $(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{2}{3})$

(4) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{5}{6})$ $0,0,z$ $(6_z^{-1}|0,0,\frac{5}{6})$

(6) $6^+(\frac{1}{6})$ $0,0,z$ $(6_z|0,0,\frac{1}{6})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	l : $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$	

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3_1$ (43) 1; 2; 3
[3] $\not{p}112_1$ (9) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [5] $\not{p}6_5$ ($\mathbf{c}'=5\mathbf{c}$) (58); [7] $\not{p}6_1$ ($\mathbf{c}'=7\mathbf{c}$) (54)

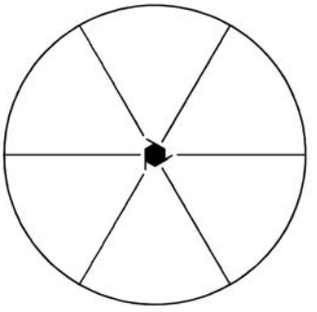
Minimal non-isotypic non-enantiomorphic supergroups

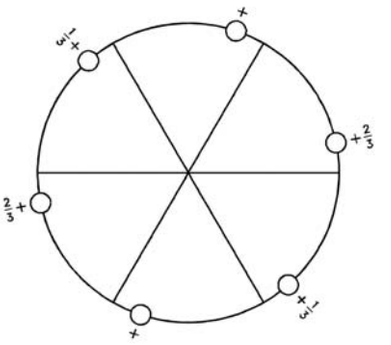
I [2] $\not{p}6_122$ (63)

II [2] $\not{p}6_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (55); [3] $\not{p}6_3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (56)

$\not p 6_2$ 6 Hexagonal

No. 55 $\not p 6_2$ Patterson symmetry $\not p 6/m$





Origin on 2 on 6_2

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$ $(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{1}{3})$

(4) 2 $0,0,z$ $(2_z|0,0,0)$

(5) $6^-(\frac{2}{3})$ $0,0,z$ $(6_z^{-1}|0,0,\frac{2}{3})$

(6) $6^+(\frac{1}{3})$ $0,0,z$ $(6_z|0,0,\frac{1}{3})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	l : $l=3n$
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{2}{3}$	(6) $x-y,x,z+\frac{1}{3}$	
				Special: no extra conditions
3 a 2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{1}\,1\,m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{1}\,1\,m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{3}_2$ (44) 1; 2; 3
[3] $\not{1}\,1\,2$ (8) 1; 4

IIa none

IIb [2] $\not{6}_1$ ($\mathbf{c}'=2\mathbf{c}$) (54)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{6}_4$ ($\mathbf{c}'=2\mathbf{c}$) (57); [7] $\not{6}_2$ ($\mathbf{c}'=7\mathbf{c}$) (55)

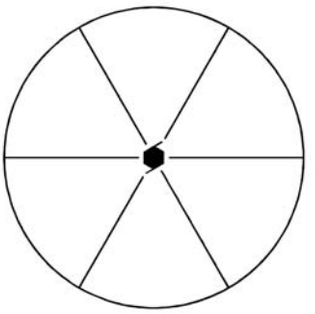
Minimal non-isotypic non-enantiomorphic supergroups

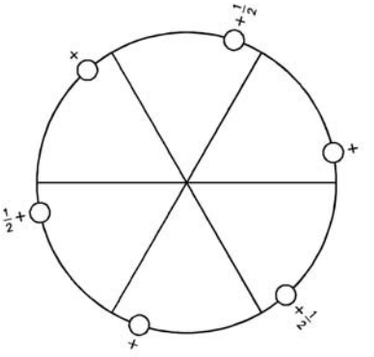
I [2] $\not{6}_2\,2\,2$ (64)

II [3] $\not{6}$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (53)

$\not p 6_3$ 6 Hexagonal

No. 56 $\not p 6_3$ Patterson symmetry $\not p 6/m$





Origin on 3 on 6_3

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2})$ $0,0,z$
$(6_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
				Special: no extra conditions
2 a 3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$		

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3$ (42) 1; 2; 3
[3] $\not{p}1\,1\,2_1$ (9) 1; 4

IIa none

IIb [3] $\not{p}6_5$ ($\mathbf{c}'=3\mathbf{c}$) (58); [3] $\not{p}6_1$ ($\mathbf{c}'=3\mathbf{c}$) (54)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}6_3$ ($\mathbf{c}'=3\mathbf{c}$) (56)

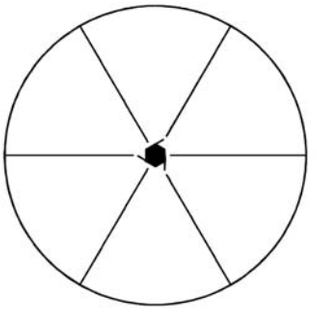
Minimal non-isotypic non-enantiomorphic supergroups

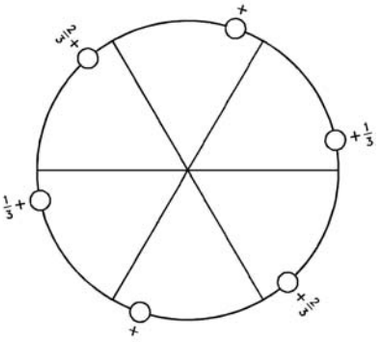
I [2] $\not{p}6_3/m$ (61); [2] $\not{p}6_3\,2\,2$ (65); [2] $\not{p}6_3\,m\,c$ (70)

II [2] $\not{p}6$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (53)

$\not p 6_4$ 6 Hexagonal

No. 57 $\not p 6_4$ Patterson symmetry $\not p 6/m$





Origin on 2 on 6_4

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$
$(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{2}{3})$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) $6^-(\frac{1}{3})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{3})$

(6) $6^+(\frac{2}{3})$ $0,0,z$
$(6_z|0,0,\frac{2}{3})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6 b 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$		General:
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{1}{3}$	(6) $x-y,x,z+\frac{2}{3}$		l : $l=3n$
					Special: no extra conditions
3 a 2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$		

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{1}\,1\,m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{1}\,1\,m$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{3}_1$ (43) 1; 2; 3
[3] $\not{1}\,1\,2$ (8) 1; 4

IIa none

IIb [2] $\not{6}_5$ ($\mathbf{c}'=2\mathbf{c}$) (58)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{6}_2$ ($\mathbf{c}'=2\mathbf{c}$) (55); [7] $\not{6}_4$ ($\mathbf{c}'=7\mathbf{c}$) (57)

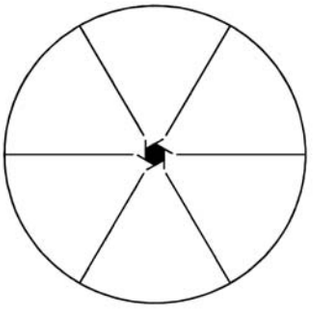
Minimal non-isotypic non-enantiomorphic supergroups

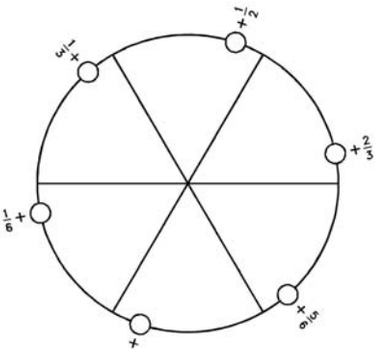
I [2] $\not{6}_4\,2\,2$ (66)

II [3] $\not{6}$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (53)

$\not p 6_5$ 6 Hexagonal

No. 58 $\not p 6_5$ Patterson symmetry $\not p 6/m$





Origin on 6_5

Asymmetric unit $0 \le z \le \frac{1}{6}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$ $(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$ $(3_z^{-1}|0,0,\frac{1}{3})$

(4) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{6})$ $0,0,z$ $(6_z^{-1}|0,0,\frac{1}{6})$

(6) $6^+(\frac{5}{6})$ $0,0,z$ $(6_z|0,0,\frac{5}{6})$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$		l : $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$		

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{P}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{P}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{P}3_2$ (44) 1; 2; 3
[3] $\not{P}1\,1\,2_1$ (9) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [5] $\not{P}6_1$ ($\mathbf{c}'=5\mathbf{c}$) (54); [7] $\not{P}6_5$ ($\mathbf{c}'=7\mathbf{c}$) (58)

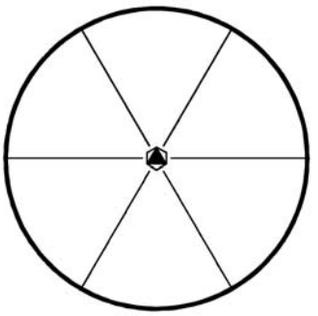
Minimal non-isotypic non-enantiomorphic supergroups

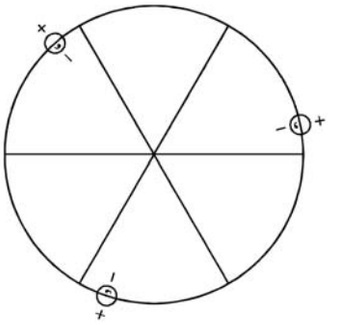
I [2] $\not{P}6_5\,2\,2$ (67)

II [2] $\not{P}6_4$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (57); [3] $\not{P}6_3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (56)

$p\bar{6}$ $\bar{6}$ Hexagonal

No. 59 $p\bar{6}$ Patterson symmetry $p6/m$





Origin at $\bar{6}$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z;$ $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z;$ $0,0,0$
$(\bar{6}_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z (4) $x,y,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$	no conditions
						Special: no extra conditions
3	e	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	
3	d	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	$\bar{6}$ . .	$0,0,\frac{1}{2}$			
1	a	$\bar{6}$ . .	$0,0,0$			

Symmetry of special projections

Along [001] 3
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1m1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}3$ (42) 1; 2; 3
[3] $\not{p}11m$ (10) 1; 4

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{6}$ ($\mathbf{c}' = 2\mathbf{c}$) (59)

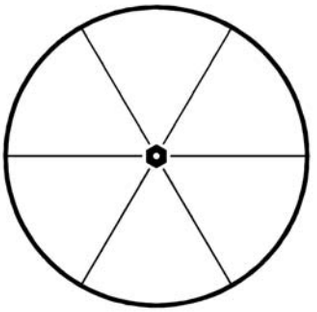
Minimal non-isotypic non-enantiomorphic supergroups

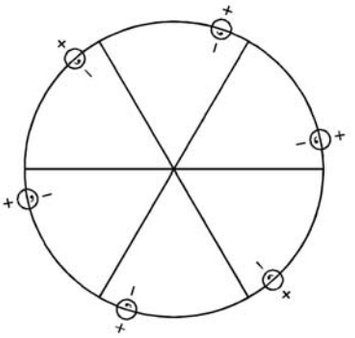
I [2] $\not{p}6/m$ (60); [2] $\not{p}6_3/m$ (61); [2] $\not{p}\bar{6}m2$ (71); [2] $\not{p}\bar{6}c2$ (72)

II none

$\not{p}6/m$ $6/m$ Hexagonal

No. 60 $\not{p}6/m$ Patterson symmetry $\not{p}6/m$





Origin at centre $(6/m)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m $x,y,0$
$(m_z|0,0,0)$

(11) $\bar{6}^-$ $0,0,z;\ 0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(12) $\bar{6}^+$ $0,0,z;\ 0,0,0$
$(\bar{6}_z|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	
			(10) $x,y,\bar{z}$	(11) $\bar{y},x-y,\bar{z}$	(12) $\bar{x}+y,\bar{x},\bar{z}$	
						Special: no extra conditions
6	e	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$
6	d	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$
2	c	6 . .	$0,0,z$	$0,0,\bar{z}$				
1	b	$6/m$ . .	$0,0,\frac{1}{2}$					
1	a	$6/m$ . .	$0,0,0$					

Symmetry of special projections

Along [001] 6
Origin at $0,0,z$

Along [100] $\not{2}mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{2}mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{6}\,\bar{6}$ (59) 1; 2; 3; 10; 11; 12
[2] $\not{6}\,6$ (53) 1; 2; 3; 4; 5; 6
[2] $\not{6}\,\bar{3}$ (45) 1; 2; 3; 7; 8; 9
[3] $\not{6}\,1\,1\,2/m$ (11) 1; 4; 7; 10

IIa none

IIb [2] $\not{6}\,6_3/m$ ($\mathbf{c}' = 2\mathbf{c}$) (61)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{6}\,6/m$ ($\mathbf{c}' = 2\mathbf{c}$) (60)

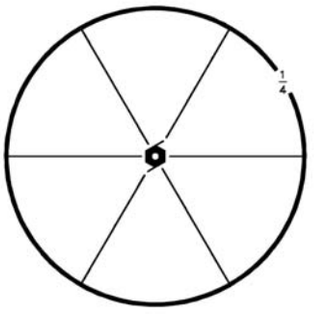
Minimal non-isotypic non-enantiomorphic supergroups

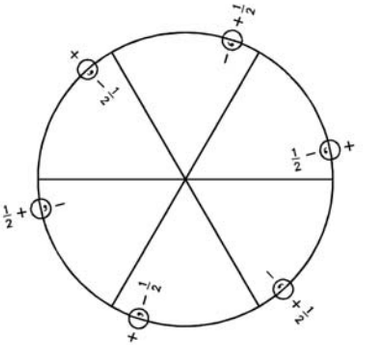
I [2] $\not{6}\,6/mmm$ (73); [2] $\not{6}\,6/mcc$ (74)

II none

$\not{p}6_3/m$ $6/m$ Hexagonal

No. 61 $\not{p}6_3/m$ Patterson symmetry $\not{p}6/m$





Origin at centre $(\bar{3})$ on 6_3

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2})$ $0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z;$ $0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z;$ $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m $x,y,\frac{1}{4}$
$(m_z|0,0,\frac{1}{2})$

(11) $\bar{6}^-$ $0,0,z;$ $0,0,\frac{1}{4}$
$(\bar{6}_z^{-1}|0,0,\frac{1}{2})$

(12) $\bar{6}^+$ $0,0,z;$ $0,0,\frac{1}{4}$
$(\bar{6}_z|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	e	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$	l : $l=2n$
						Special: no extra conditions
6	d	m . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$
4	c	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$		
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$				
2	a	$\bar{6}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				

Symmetry of special projections

Along [001] 6	Along [100] $\not{2}mg$	Along [210] $\not{2}mg$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{6}$ (59)	1; 2; 3; 10; 11; 12
	[2] $\not{6}_3$ (56)	1; 2; 3; 4; 5; 6
	[2] $\not{\bar{3}}$ (45)	1; 2; 3; 7; 8; 9
	[3] $\not{1}\,1\,2_1/m$ (12)	1; 4; 7; 10
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{6}_3/m$ ($\mathbf{c}'=3\mathbf{c}$) (61)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\not{6}_3/mmc$ (75)

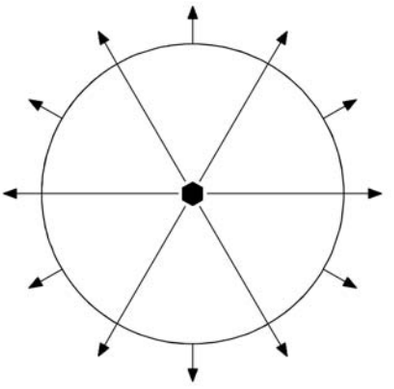
II [2] $\not{6}/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (60)

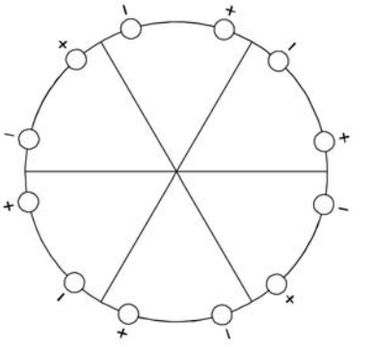
International Tables for Crystallography (2010). Vol. E, Rod group 62, pp. 184–185.

$p622$ 622 Hexagonal

No. 62 $p622$

Patterson symmetry $p6/mmm$





Origin at 622

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	h	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}$				no conditions
									Special: no extra conditions
6	g	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	
6	f	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
6	e	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	d	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
2	c	6 . .	$0,0,z$	$0,0,\bar{z}$					
1	b	6 2 2	$0,0,\frac{1}{2}$						
1	a	6 2 2	$0,0,0$						

Symmetry of special projections

Along [001] $6mm$	Along [100] $\not{p}2mm$	Along [210] $\not{p}2mm$
	$\mathbf{a}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}6\,1\,1$ ($\not{p}6$, 53)	1; 2; 3; 4; 5; 6
	[2] $\not{p}3\,2\,1$ ($\not{p}3\,1\,2$, 46)	1; 2; 3; 7; 8; 9
	[2] $\not{p}3\,1\,2$ (46)	1; 2; 3; 10; 11; 12
	[3] $\not{p}2\,2\,2$ ($\not{p}2\,2\,2$, 13)	1; 4; 7; 10
	[3] $\not{p}2\,2\,2$ ($\not{p}2\,2\,2$, 13)	1; 4; 8; 11
	[3] $\not{p}2\,2\,2$ ($\not{p}2\,2\,2$, 13)	1; 4; 9; 12
IIa	none	
IIb	[2] $\not{p}6_3\,2\,2$ ($\mathbf{c}' = 2\mathbf{c}$) (65); [3] $\not{p}6_4\,2\,2$ ($\mathbf{c}' = 3\mathbf{c}$) (66); [3] $\not{p}6_2\,2\,2$ ($\mathbf{c}' = 3\mathbf{c}$) (64)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}6\,2\,2$ ($\mathbf{c}' = 2\mathbf{c}$) (62)

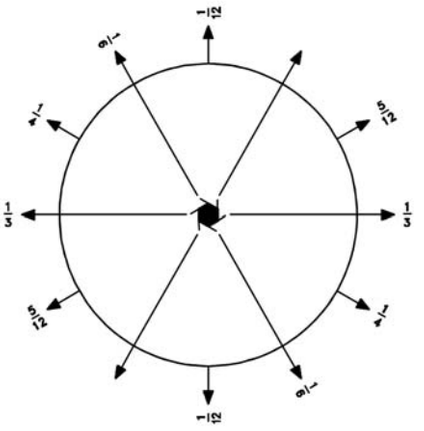
Minimal non-isotypic non-enantiomorphic supergroups

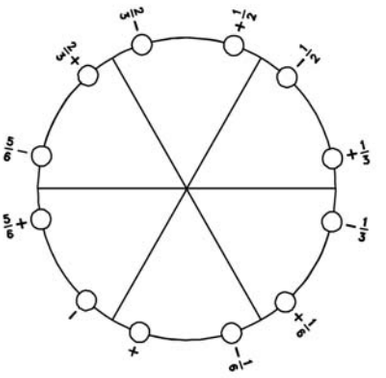
I [2] $\not{p}6/mmm$ (73); [2] $\not{p}6/mcc$ (74)

II none

$\not{p}6_1 22$ 622 Hexagonal

No. 63 $\not{p}6_1 22$ Patterson symmetry $\not{p}6/mmm$





Origin on $2[100]$ at $6_1(2,1,1)1$

Asymmetric unit $0 \le z \le \frac{1}{12}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$
$(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{2}{3})$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{5}{6})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{5}{6})$

(6) $6^+(\frac{1}{6})$ $0,0,z$
$(6_z|0,0,\frac{1}{6})$

(7) 2 $x,x,\frac{1}{6}$
$(2_{xy}|0,0,\frac{1}{3})$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,\frac{1}{3}$
$(2_y|0,0,\frac{2}{3})$

(10) 2 $x,\bar{x},\frac{5}{12}$
$(2_3|0,0,\frac{5}{6})$

(11) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) 2 $2x,x,\frac{1}{12}$
$(2_1|0,0,\frac{1}{6})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	c	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{3}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{5}{6}$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $y,\bar{x}+y,z+\frac{5}{6}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $x-y,x,z+\frac{1}{6}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$ (12) $x,x-y,\bar{z}+\frac{1}{6}$				l : $l=6n$
									Special: as above, plus
6	b	. . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{7}{12}$	$x,\bar{x},\frac{11}{12}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{1}{12}$	$\bar{x},x,\frac{5}{12}$	l : $l=2n$ or $l=3n+1$ or $l=3n+2$
6	a	. 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{5}{6}$	$x,x,\frac{1}{6}$	l : $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $P2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $P2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{12}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P6_111$ ($P6_1$, 54) 1; 2; 3; 4; 5; 6
[2] $P3_121$ ($P3_112$, 47) 1; 2; 3; 7; 8; 9
[2] $P3_112$ (47) 1; 2; 3; 10; 11; 12
[3] $P2_122$ ($P222_1$, 14) 1; 4; 7; 10
[3] $P2_122$ ($P222_1$, 14) 1; 4; 8; 11
[3] $P2_122$ ($P222_1$, 14) 1; 4; 9; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [5] $P6_522$ ($\mathbf{c}'=5\mathbf{c}$) (67); [7] $P6_122$ ($\mathbf{c}'=7\mathbf{c}$) (63)

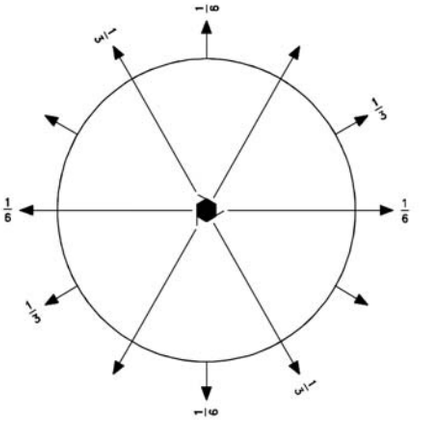
Minimal non-isotypic non-enantiomorphic supergroups

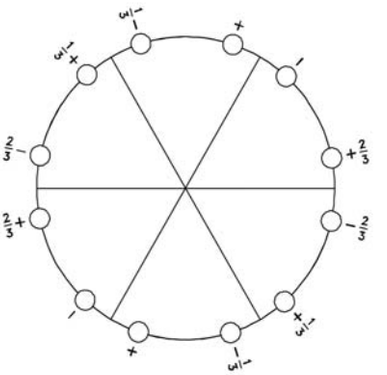
I none

II [2] $P6_222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (64); [3] $P6_322$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (65)

$\not p 6_2 22$ 622 Hexagonal

No. 64 $\not p 6_2 22$ Patterson symmetry $\not p 6/mmm$





Origin on 222 at $6_2(2,1,1)(1,2,1)$

Asymmetric unit $0 \le x; \quad 0 \le z \le \frac{1}{6}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$
$(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{1}{3})$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) $6^-(\frac{2}{3})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{2}{3})$

(6) $6^+(\frac{1}{3})$ $0,0,z$
$(6_z|0,0,\frac{1}{3})$

(7) 2 $x,x,\frac{1}{3}$
$(2_{xy}|0,0,\frac{2}{3})$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,\frac{1}{6}$
$(2_y|0,0,\frac{1}{3})$

(10) 2 $x,\bar{x},\frac{1}{3}$
$(2_3|0,0,\frac{2}{3})$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,\frac{1}{6}$
$(2_1|0,0,\frac{1}{3})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	h	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	l : $l=3n$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{2}{3}$	(6) $x-y,x,z+\frac{1}{3}$	
			(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	
			(10) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}+\frac{1}{3}$	
						Special: no extra conditions
6	g	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{6}$	$x,\bar{x},\frac{5}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$ $2x,x,\frac{1}{6}$ $\bar{x},x,\frac{5}{6}$
6	f	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{2}{3}$	$x,\bar{x},\frac{1}{3}$	$\bar{x},2\bar{x},0$ $2x,x,\frac{2}{3}$ $\bar{x},x,\frac{1}{3}$
6	e	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{5}{6}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{6}$ $x,x,\frac{5}{6}$
6	d	. 2 .	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,0$ $0,\bar{x},\frac{2}{3}$ $x,x,\frac{1}{3}$
6	c	2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	$0,0,\bar{z}+\frac{2}{3}$ $0,0,\bar{z}$ $0,0,\bar{z}+\frac{1}{3}$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{1}{6}$	$0,0,\frac{5}{6}$	
3	a	2 2 2	$0,0,0$	$0,0,\frac{2}{3}$	$0,0,\frac{1}{3}$	

Symmetry of special projections

Along [001] $6mm$	Along [100] $\not{p}2mm$	Along [210] $\not{p}2mm$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,\frac{1}{6}$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}6_2 11$ ($\not{p}6_2$, 55)	1; 2; 3; 4; 5; 6
	[2] $\not{p}3_2 21$ ($\not{p}3_2 12$, 48)	1; 2; 3; 7; 8; 9
	[2] $\not{p}3_2 12$ (48)	1; 2; 3; 10; 11; 12
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 7; 10
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 8; 11
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 9; 12
IIa	none	
IIb	[2] $\not{p}6_1 22$ ($\mathbf{c}'=2\mathbf{c}$) (63)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}6_4 22$ ($\mathbf{c}'=2\mathbf{c}$) (66); [7] $\not{p}6_2 22$ ($\mathbf{c}'=7\mathbf{c}$) (64)

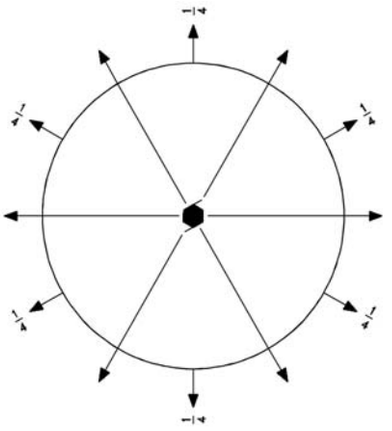
Minimal non-isotypic non-enantiomorphic supergroups

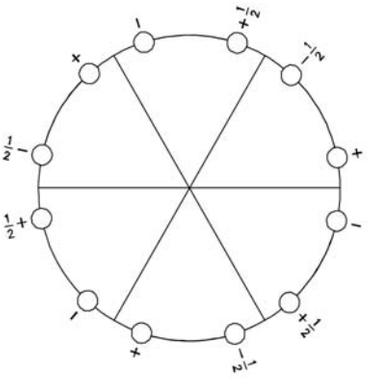
I none

II [3] $\not{p}622$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (62)

$\not p 6_3 22$ 622 Hexagonal

No. 65 $\not p 6_3 22$ Patterson symmetry $\not p 6/mmm$





Origin at 321 at $6_3 21$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+ \; 0,0,z$
$(3_z|0,0,0)$

(3) $3^- \; 0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2}) \; 0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2}) \; 0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2}) \; 0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) $2 \; x,x,0$
$(2_{xy}|0,0,0)$

(8) $2 \; x,0,0$
$(2_x|0,0,0)$

(9) $2 \; 0,y,0$
$(2_y|0,0,0)$

(10) $2 \; x,\bar{x},\frac{1}{4}$
$(2_3|0,0,\frac{1}{2})$

(11) $2 \; x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) $2 \; 2x,x,\frac{1}{4}$
$(2_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$	
						Special: no extra conditions
6	e	. . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$
6	d	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$
4	c	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$		
2	b	3 . 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				
2	a	3 2 .	$0,0,0$	$0,0,\frac{1}{2}$				

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{4}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}6_3 11$ ($\not{p}6_3$, 56) 1; 2; 3; 4; 5; 6
[2] $\not{p}321$ ($\not{p}312$, 46) 1; 2; 3; 7; 8; 9
[2] $\not{p}312$ (46) 1; 2; 3; 10; 11; 12
[3] $\not{p}2_122$ ($\not{p}222_1$, 14) 1; 4; 7; 10
[3] $\not{p}2_122$ ($\not{p}222_1$, 14) 1; 4; 8; 11
[3] $\not{p}2_122$ ($\not{p}222_1$, 14) 1; 4; 9; 12

IIa none

IIb [3] $\not{p}6_522$ ($\mathbf{c}'=3\mathbf{c}$) (67); [3] $\not{p}6_122$ ($\mathbf{c}'=3\mathbf{c}$) (63)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}6_322$ ($\mathbf{c}'=3\mathbf{c}$) (65)

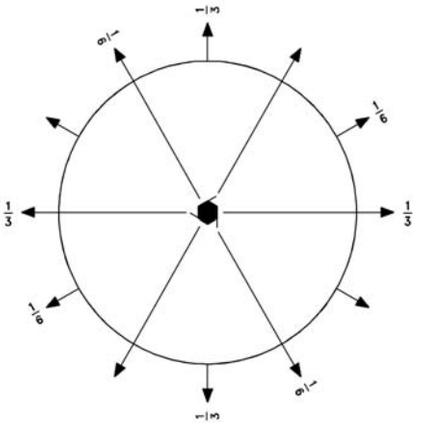
Minimal non-isotypic non-enantiomorphic supergroups

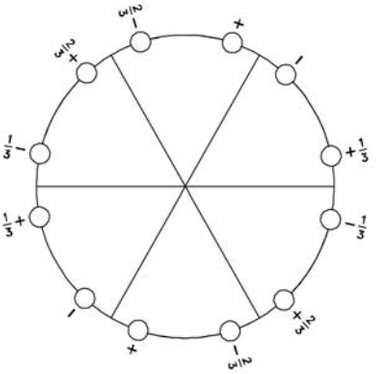
I [2] $\not{p}6_3/mmc$ (75)

II [2] $\not{p}622$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (62)

$\not p 6_4 22$ 622 Hexagonal

No. 66 $\not p 6_4 22$ Patterson symmetry $\not p 6/mmm$





Origin on 222 at $6_4(2,1,1)(1,2,1)$

Asymmetric unit $0 \le x; \quad 0 \le z \le \frac{1}{6}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{1}{3})$ $0,0,z$
$(3_z|0,0,\frac{1}{3})$

(3) $3^-(\frac{2}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{2}{3})$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) $6^-(\frac{1}{3})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{3})$

(6) $6^+(\frac{2}{3})$ $0,0,z$
$(6_z|0,0,\frac{2}{3})$

(7) 2 $x,x,\frac{1}{6}$
$(2_{xy}|0,0,\frac{1}{3})$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,\frac{1}{3}$
$(2_y|0,0,\frac{2}{3})$

(10) 2 $x,\bar{x},\frac{1}{6}$
$(2_3|0,0,\frac{1}{3})$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,\frac{1}{3}$
$(2_1|0,0,\frac{2}{3})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	h	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	l : $l=3n$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{1}{3}$	(6) $x-y,x,z+\frac{2}{3}$	
			(7) $y,x,\bar{z}+\frac{1}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}+\frac{2}{3}$	
						Special: no extra conditions
6	g	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{5}{6}$	$x,\bar{x},\frac{1}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{5}{6}$	$\bar{x},x,\frac{1}{6}$
6	f	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{1}{3}$	$x,\bar{x},\frac{2}{3}$	$\bar{x},2\bar{x},0$	$2x,x,\frac{1}{3}$	$\bar{x},x,\frac{2}{3}$
6	e	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{6}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{5}{6}$	$x,x,\frac{1}{6}$
6	d	. 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,0$	$0,\bar{x},\frac{1}{3}$	$x,x,\frac{2}{3}$
6	c	2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$	$0,0,\bar{z}+\frac{1}{3}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{2}{3}$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{5}{6}$	$0,0,\frac{1}{6}$			
3	a	2 2 2	$0,0,0$	$0,0,\frac{1}{3}$	$0,0,\frac{2}{3}$			

Symmetry of special projections

Along [001] $6mm$	Along [100] $\not{p}2mm$	Along [210] $\not{p}2mm$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,\frac{1}{3}$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}6_4 11$ ($\not{p}6_4$, 57)	1; 2; 3; 4; 5; 6
	[2] $\not{p}3_1 21$ ($\not{p}3_1 12$, 47)	1; 2; 3; 7; 8; 9
	[2] $\not{p}3_1 12$ (47)	1; 2; 3; 10; 11; 12
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 7; 10
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 8; 11
	[3] $\not{p}222$ ($\not{p}222$, 13)	1; 4; 9; 12
IIa	none	
IIb	[2] $\not{p}6_5 22$ ($\mathbf{c}'=2\mathbf{c}$) (67)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}6_2 22$ ($\mathbf{c}'=2\mathbf{c}$) (64); [7] $\not{p}6_4 22$ ($\mathbf{c}'=7\mathbf{c}$) (66)

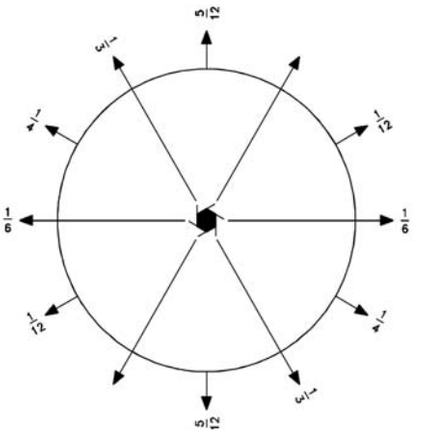
Minimal non-isotypic non-enantiomorphic supergroups

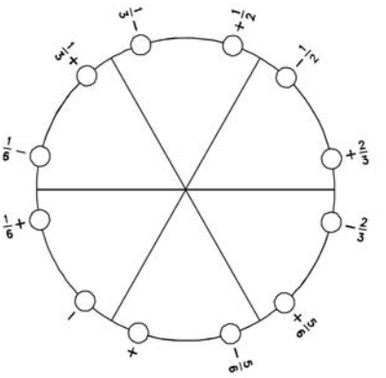
I none

II [3] $\not{p}622$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (62)

$\not{p}6_522$ 622 Hexagonal

No. 67 $\not{p}6_522$ Patterson symmetry $\not{p}6/mmm$





Origin on $2[100]$ at $6_5(2,1,1)1$

Asymmetric unit $0 \le z \le \frac{1}{12}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+(\frac{2}{3})$ $0,0,z$
$(3_z|0,0,\frac{2}{3})$

(3) $3^-(\frac{1}{3})$ $0,0,z$
$(3_z^{-1}|0,0,\frac{1}{3})$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{6})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{6})$

(6) $6^+(\frac{5}{6})$ $0,0,z$
$(6_z|0,0,\frac{5}{6})$

(7) 2 $x,x,\frac{1}{3}$
$(2_{xy}|0,0,\frac{2}{3})$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,\frac{1}{6}$
$(2_y|0,0,\frac{1}{3})$

(10) 2 $x,\bar{x},\frac{1}{12}$
$(2_3|0,0,\frac{1}{6})$

(11) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) 2 $2x,x,\frac{5}{12}$
$(2_1|0,0,\frac{5}{6})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$				l : $l=6n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$				
			(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{5}{6}$				
									Special: as above, plus
6	b	. . 2	$x,2x,\frac{3}{4}$	$2\bar{x},\bar{x},\frac{5}{12}$	$x,\bar{x},\frac{1}{12}$	$\bar{x},2\bar{x},\frac{1}{4}$	$2x,x,\frac{11}{12}$	$\bar{x},x,\frac{7}{12}$	l : $l=2n$ or $l=3n+1$ or $l=3n+2$
6	a	. 2 .	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{6}$	$x,x,\frac{5}{6}$	l : $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $6mm$	Along [100] $P2mg$	Along [210] $P2mg$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,\frac{5}{12}$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $P6_511$ ($P6_5$, 58)	1; 2; 3; 4; 5; 6
	[2] $P3_221$ ($P3_212$, 48)	1; 2; 3; 7; 8; 9
	[2] $P3_212$ (48)	1; 2; 3; 10; 11; 12
	[3] $P2_122$ ($P222_1$, 14)	1; 4; 7; 10
	[3] $P2_122$ ($P222_1$, 14)	1; 4; 8; 11
	[3] $P2_122$ ($P222_1$, 14)	1; 4; 9; 12
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [5] $P6_122$ ($\mathbf{c}'=5\mathbf{c}$) (63); [7] $P6_522$ ($\mathbf{c}'=7\mathbf{c}$) (67)

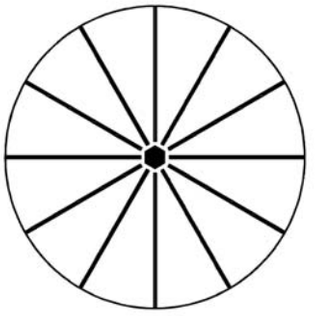
Minimal non-isotypic non-enantiomorphic supergroups

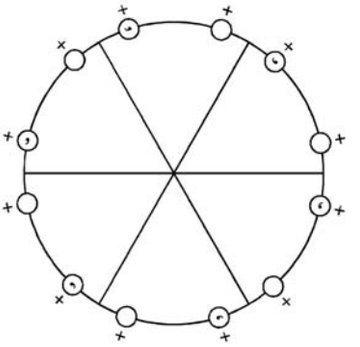
I none

II [2] $P6_422$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (66); [3] $P6_322$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (65)

$\not{p}6mm$ $6mm$ Hexagonal

No. 68 $\not{p}6mm$ Patterson symmetry $\not{p}6/mmm$





Origin on $6mm$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x/2$

Symmetry operations

(1) 1 $(1\|0,0,0)$	(2) 3^+ $0,0,z$ $(3_z\|0,0,0)$	(3) 3^- $0,0,z$ $(3_z^{-1}\|0,0,0)$
(4) 2 $0,0,z$ $(2_z\|0,0,0)$	(5) 6^- $0,0,z$ $(6_z^{-1}\|0,0,0)$	(6) 6^+ $0,0,z$ $(6_z\|0,0,0)$
(7) m $x,\bar{x},z$ $(m_{xy}\|0,0,0)$	(8) m $x,2x,z$ $(m_x\|0,0,0)$	(9) m $2x,x,z$ $(m_y\|0,0,0)$
(10) m x,x,z $(m_3\|0,0,0)$	(11) m $x,0,z$ $(m_2\|0,0,0)$	(12) m $0,y,z$ $(m_1\|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$	
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
6	c	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z$ $\bar{x},2\bar{x},z$ $2x,x,z$
6	b	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$ $0,\bar{x},z$ x,x,z
1	a	$6mm$	$0,0,z$			

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}11m$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}611$ ($\not{p}6$, 53) 1; 2; 3; 4; 5; 6
[2] $\not{p}3m1$ (49) 1; 2; 3; 7; 8; 9
[2] $\not{p}31m$ ($\not{p}3m1$, 49) 1; 2; 3; 10; 11; 12
[3] $\not{p}2mm$ ($\not{p}mm2$, 15) 1; 4; 7; 10
[3] $\not{p}2mm$ ($\not{p}mm2$, 15) 1; 4; 8; 11
[3] $\not{p}2mm$ ($\not{p}mm2$, 15) 1; 4; 9; 12

IIa none

IIb [2] $\not{p}6_3mc$ ($\mathbf{c}' = 2\mathbf{c}$) (70); [2] $\not{p}6_3cm$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}6_3mc$, 70); [2] $\not{p}6cc$ ($\mathbf{c}' = 2\mathbf{c}$) (69)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}6mm$ ($\mathbf{c}' = 2\mathbf{c}$) (68)

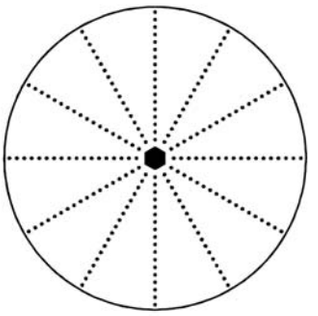
Minimal non-isotypic non-enantiomorphic supergroups

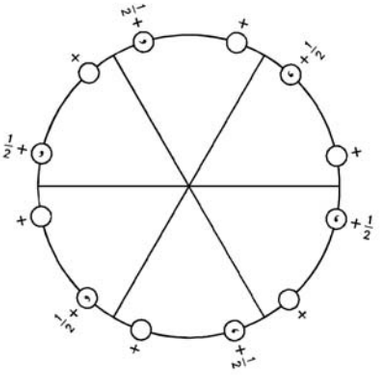
I [2] $\not{p}6/mmm$ (73)

II none

$\not{p}6cc$ $6mm$ Hexagonal

No. 69 $\not{p}6cc$ Patterson symmetry $\not{p}6/mmm$





Origin on $6cc$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c $x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(9) c $2x,x,z$
$(m_y|0,0,\frac{1}{2})$

(10) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(11) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(12) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
12 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$		l : $l=2n$
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$		
	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$		
	(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$		
					Special: no extra conditions
2 a 6 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}611$ ($\not{p}6$, 53)	1; 2; 3; 4; 5; 6
	[2] $\not{p}3c1$ (50)	1; 2; 3; 7; 8; 9
	[2] $\not{p}31c$ ($\not{p}3c1$, 50)	1; 2; 3; 10; 11; 12
	[3] $\not{p}2cc$ ($\not{p}cc2$, 16)	1; 4; 7; 10
	[3] $\not{p}2cc$ ($\not{p}cc2$, 16)	1; 4; 8; 11
	[3] $\not{p}2cc$ ($\not{p}cc2$, 16)	1; 4; 9; 12
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}6cc$ ($\mathbf{c}'=3\mathbf{c}$) (69)

Minimal non-isotypic non-enantiomorphic supergroups

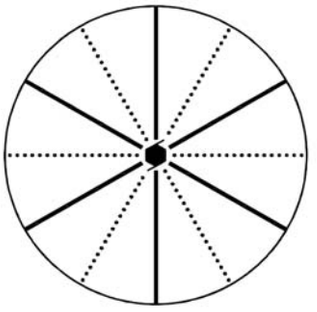
I [2] $\not{p}6/mcc$ (74)

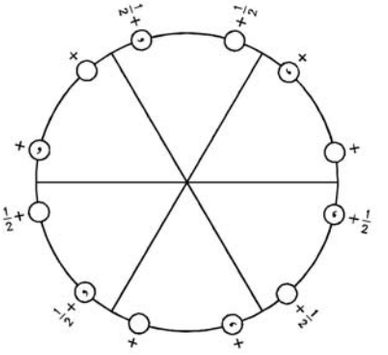
II [2] $\not{p}6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (68)

$\not{p}6_3mc$ $6mm$ Hexagonal

No. 70 $\not{p}6_3mc$ Patterson symmetry $\not{p}6/mmm$

FIRST SETTING





Origin on $3m1$ on 6_3mc

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x/2$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2})$ $0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m $x,2x,z$
$(m_x|0,0,0)$

(9) m $2x,x,z$
$(m_y|0,0,0)$

(10) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(11) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(12) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$	
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	
						Special: no extra conditions
6	b	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$ $\bar{x},2\bar{x},z+\frac{1}{2}$ $2x,x,z+\frac{1}{2}$
2	a	3 m .	$0,0,z$	$0,0,z+\frac{1}{2}$		

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}1\,1\,g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}6_3\,1\,1$ ($\not{p}6_3$, 56)	1; 2; 3; 4; 5; 6
	[2] $\not{p}3\,1\,c$ ($\not{p}3\,c\,1$, 50)	1; 2; 3; 10; 11; 12
	[2] $\not{p}3\,m\,1$ (49)	1; 2; 3; 7; 8; 9
	[3] $\not{p}2_1\,mc$ ($\not{p}mc2_1$, 17)	1; 4; 7; 10
	[3] $\not{p}2_1\,mc$ ($\not{p}mc2_1$, 17)	1; 4; 8; 11
	[3] $\not{p}2_1\,mc$ ($\not{p}mc2_1$, 17)	1; 4; 9; 12
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}6_3mc$ ($\mathbf{c}'=3\mathbf{c}$) (70)

Minimal non-isotypic non-enantiomorphic supergroups

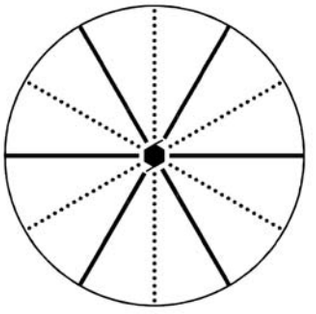
I [2] $\not{p}6_3/mmc$ (75)

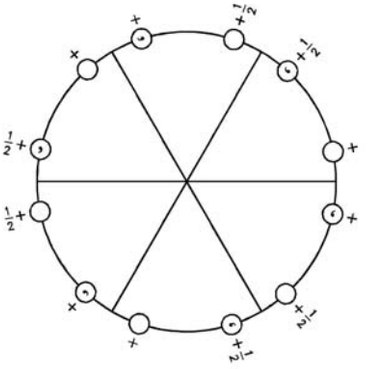
II [2] $\not{p}6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (68)

No. 70 $\not{p}6_3cm$

Patterson symmetry $\not{p}6/mmm$

SECOND SETTING





Origin on $31m$ on 6_3cm

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le 1; \quad y \le x/2$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2})$ $0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c $x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(9) c $2x,x,z$
$(m_y|0,0,\frac{1}{2})$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$	
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
6	b	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$ $0,\bar{x},z+\frac{1}{2}$ $x,x,z+\frac{1}{2}$
2	a	$3.m$	$0,0,z$	$0,0,z+\frac{1}{2}$		

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{P}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{P}11g$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{P}6_311$ ($\not{P}6_3$, 56)	1; 2; 3; 4; 5; 6
	[2] $\not{P}3c1$ (50)	1; 2; 3; 7; 8; 9
	[2] $\not{P}31m$ ($\not{P}3m1$, 49)	1; 2; 3; 10; 11; 12
	[3] $\not{P}2_1cm$ ($\not{P}mc2_1$, 17)	1; 4; 7; 10
	[3] $\not{P}2_1cm$ ($\not{P}mc2_1$, 17)	1; 4; 8; 11
	[3] $\not{P}2_1cm$ ($\not{P}mc2_1$, 17)	1; 4; 9; 12
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{P}6_3cm$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{P}6_3mc$, 70)

Minimal non-isotypic non-enantiomorphic supergroups

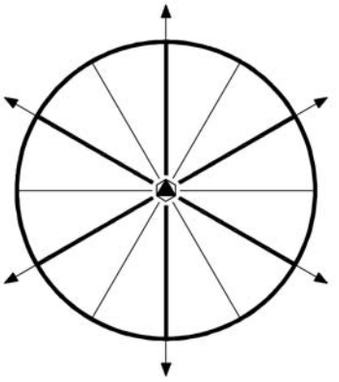
I [2] $\not{P}6_3/mmc$ (75)

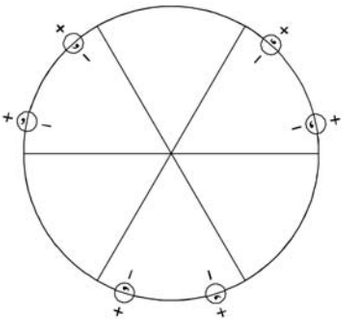
II [2] $\not{P}6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (68)

$\not{p}\bar{6}m2$ $\bar{6}m2$ Hexagonal

No. 71 $\not{p}\bar{6}m2$ Patterson symmetry $\not{p}6/mmm$

FIRST SETTING





Origin on $\bar{6}m2$

Asymmetric unit $y \le x/2; \quad -x \le y; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z;$ $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z;$ $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m $x,2x,z$
$(m_x|0,0,0)$

(9) m $2x,x,z$
$(m_y|0,0,0)$

(10) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$				
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$				
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$				
									Special: no extra conditions
6	h	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$x,2x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}$	
6	g	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	$\bar{x}+y,y,\frac{1}{2}$	$x,x-y,\frac{1}{2}$	
6	f	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{y},\bar{x},0$	$\bar{x}+y,y,0$	$x,x-y,0$	
3	e	$m\,m\,2$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$				
3	d	$m\,m\,2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$				
2	c	$3\,m$.	$0,0,z$	$0,0,\bar{z}$					
1	b	$\bar{6}\,m\,2$	$0,0,\frac{1}{2}$						
1	a	$\bar{6}\,m\,2$	$0,0,0$						

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}\bar{6}11$ ($\not{p}\bar{6}$, 59) 1; 2; 3; 4; 5; 6
[2] $\not{p}3m1$ (49) 1; 2; 3; 7; 8; 9
[2] $\not{p}312$ (46) 1; 2; 3; 10; 11; 12
[3] $\not{p}mm2$ ($\not{p}2mm$, 18) 1; 4; 7; 10
[3] $\not{p}mm2$ ($\not{p}2mm$, 18) 1; 4; 8; 11
[3] $\not{p}mm2$ ($\not{p}2mm$, 18) 1; 4; 9; 12

IIa none

IIb [2] $\not{p}\bar{6}c2$ ($\mathbf{c}' = 2\mathbf{c}$) (72)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{6}m2$ ($\mathbf{c}' = 2\mathbf{c}$) (71)

Minimal non-isotypic non-enantiomorphic supergroups

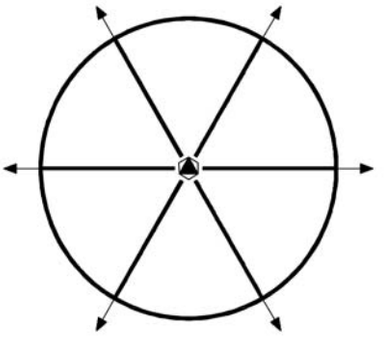
I [2] $\not{p}6/mmm$ (73); [2] $\not{p}6_3/mmc$ (75)

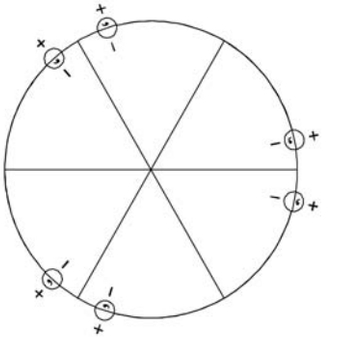
II none

No. 71 $\not{p}\bar{6}2m$

Patterson symmetry $\not{p}6/mmm$

SECOND SETTING





Origin on $\bar{6}2m$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z$; $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
6	h	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	
6	g	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	
6	f	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$x,0,\bar{z}$	$0,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
3	e	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$				
3	d	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$				
2	c	3 . m	$0,0,z$	$0,0,\bar{z}$					
1	b	$\bar{6}\,2\,m$	$0,0,\frac{1}{2}$						
1	a	$\bar{6}\,2\,m$	$0,0,0$						

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}1m1$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\not{p}\bar{6}11$ ($\not{p}\bar{6}$, 59) 1; 2; 3; 4; 5; 6
[2] $\not{p}31m$ ($\not{p}3m1$, 49) 1; 2; 3; 10; 11; 12
[2] $\not{p}321$ ($\not{p}312$, 46) 1; 2; 3; 7; 8; 9
[3] $\not{p}m2m$ ($\not{p}2mm$, 18) 1; 4; 7; 10
[3] $\not{p}m2m$ ($\not{p}2mm$, 18) 1; 4; 8; 11
[3] $\not{p}m2m$ ($\not{p}2mm$, 18) 1; 4; 9; 12

IIa none

IIb [2] $\not{p}\bar{6}2c$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{6}c2$, 72)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{p}\bar{6}2m$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{p}\bar{6}m2$, 71)

Minimal non-isotypic non-enantiomorphic supergroups

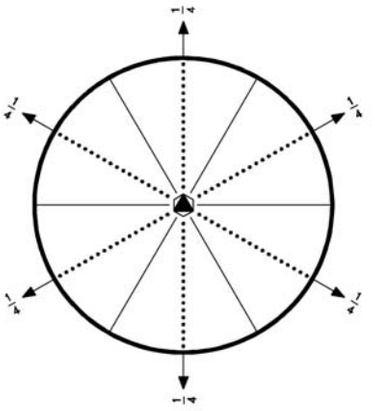
I [2] $\not{p}6/mmm$ (73); [2] $\not{p}6_3/mmc$ (75)

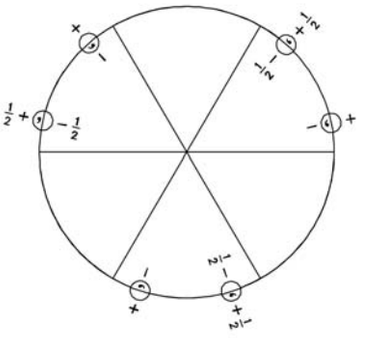
II none

$\not{p}\bar{6}c2$ $\bar{6}m2$ Hexagonal

No. 72 $\not{p}\bar{6}c2$ Patterson symmetry $\not{p}6/mmm$

FIRST SETTING





Origin on $\bar{6}c1$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z;$ $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z;$ $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(8) c $x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(9) c $2x,x,z$
$(m_y|0,0,\frac{1}{2})$

(10) 2 $x,\bar{x},\frac{1}{4}$
$(2_3|0,0,\frac{1}{2})$

(11) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) 2 $2x,x,\frac{1}{4}$
$(2_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z (4) $x,y,\bar{z}$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$ (8) $\bar{x}+y,y,z+\frac{1}{2}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$ (9) $x,x-y,z+\frac{1}{2}$ (12) $x,x-y,\bar{z}+\frac{1}{2}$	l : $l=2n$
						Special: no extra conditions
6	e	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{y},\bar{x},\frac{1}{2}$ $\bar{x}+y,y,\frac{1}{2}$ $x,x-y,\frac{1}{2}$
6	d	. . 2	$x,\bar{x},\frac{1}{4}$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$ $x,2x,\frac{3}{4}$ $2\bar{x},\bar{x},\frac{3}{4}$
4	c	3 . .	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$
2	b	$\bar{6}$ . .	$0,0,0$	$0,0,\frac{1}{2}$		
2	a	3 . 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$		

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mg$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{4}$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P\bar{6}11$ ($P\bar{6}$, 59) 1; 2; 3; 4; 5; 6
[2] $P3c1$ (50) 1; 2; 3; 7; 8; 9
[2] $P312$ (46) 1; 2; 3; 10; 11; 12
[3] $Pmc2$ ($P2cm$, 19) 1; 4; 7; 10
[3] $Pmc2$ ($P2cm$, 19) 1; 4; 8; 11
[3] $Pmc2$ ($P2cm$, 19) 1; 4; 9; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P\bar{6}c2$ ($\mathbf{c}' = 3\mathbf{c}$) (72)

Minimal non-isotypic non-enantiomorphic supergroups

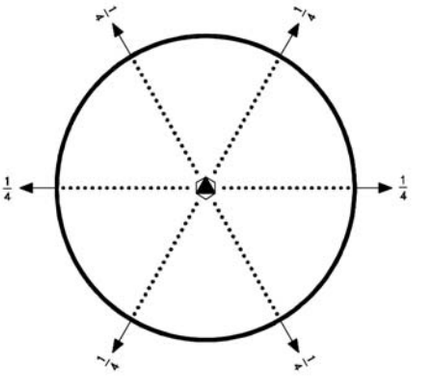
I [2] $P6/mcc$ (74); [2] $P6_3/mmc$ (75)

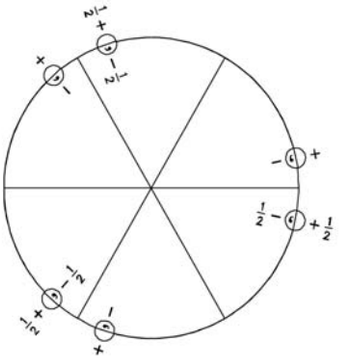
II [2] $P\bar{6}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (71)

No. 72 $p\bar{6}2c$

Patterson symmetry $p6/mmm$

SECOND SETTING





Origin on $\bar{6}1c$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z;$ $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z;$ $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) 2 $x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) 2 $x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(9) 2 $0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(10) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(11) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(12) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

Generators selected (1); $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z (4) $x,y,\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (10) $y,x,z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$ (8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ (11) $x-y,\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ (12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	l : $l=2n$
						Special: no extra conditions
6	e	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$y,x,\frac{1}{2}$ $x-y,\bar{y},\frac{1}{2}$ $\bar{x},\bar{x}+y,\frac{1}{2}$
6	d	. 2 .	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,0,\frac{3}{4}$ $0,x,\frac{3}{4}$ $\bar{x},\bar{x},\frac{3}{4}$
4	c	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$
2	b	$\bar{6}$ . .	$0,0,0$	$0,0,\frac{1}{2}$		
2	a	3 2 .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$		

Symmetry of special projections

Along [001] $3m$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $P\bar{6}11$ ($P\bar{6}$, 59) 1; 2; 3; 4; 5; 6
[2] $P31c$ ($P3c1$, 50) 1; 2; 3; 10; 11; 12
[2] $P321$ ($P312$, 46) 1; 2; 3; 7; 8; 9
[3] $Pm2c$ ($P2cm$, 19) 1; 4; 7; 10
[3] $Pm2c$ ($P2cm$, 19) 1; 4; 8; 11
[3] $Pm2c$ ($P2cm$, 19) 1; 4; 9; 12

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P\bar{6}2c$ ($\mathbf{c}'=3\mathbf{c}$) ($P\bar{6}c2$, 72)

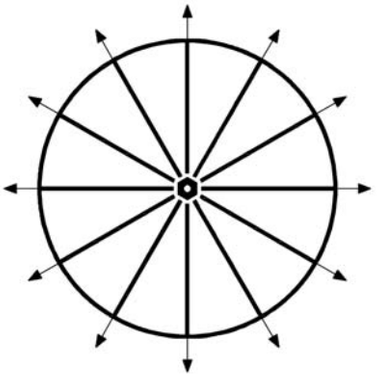
Minimal non-isotypic non-enantiomorphic supergroups

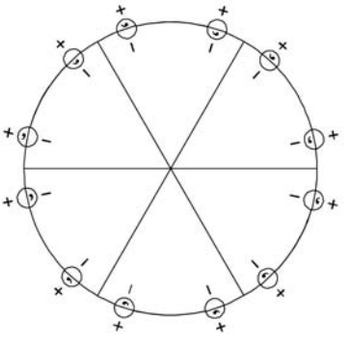
I [2] $P6/mcc$ (74); [2] $P6_3/mmc$ (75)

II [2] $P\bar{6}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (71)

$\not{6}/mmm$ $6/mmm$ Hexagonal

No. 73 $\not{6}/m2/m2/m$ Patterson symmetry $\not{6}/mmm$





Origin at centre $(6/mmm)$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{2}; \quad y \le x/2$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,0$
$(2_1|0,0,0)$

(13) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(14) $\bar{3}^+$ $0,0,z;$ $0,0,0$
$(\bar{3}_z|0,0,0)$

(15) $\bar{3}^-$ $0,0,z;$ $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(16) m $x,y,0$
$(m_z|0,0,0)$

(17) $\bar{6}^-$ $0,0,z;$ $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(18) $\bar{6}^+$ $0,0,z;$ $0,0,0$
$(\bar{6}_z|0,0,0)$

(19) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(20) m $x,2x,z$
$(m_x|0,0,0)$

(21) m $2x,x,z$
$(m_y|0,0,0)$

(22) m x,x,z
$(m_3|0,0,0)$

(23) m $x,0,z$
$(m_2|0,0,0)$

(24) m $0,y,z$
$(m_1|0,0,0)$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z$			no conditions
			(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$			
			(9) $\bar{x},\bar{x}+y,\bar{z}$	(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$			
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}$			
			(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$	(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$			
			(21) $x,x-y,z$	(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$			
									Special: no extra conditions
12	k	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$	
			$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	$\bar{x}+y,y,\frac{1}{2}$	$x,x-y,\frac{1}{2}$	
12	j	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$	
			$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	$\bar{y},\bar{x},0$	$\bar{x}+y,y,0$	$x,x-y,0$	
12	i	. m .	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z$	$2x,x,z$	$\bar{x},x,z$	
			$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}$	$x,2x,\bar{z}$	$x,\bar{x},\bar{z}$	
12	h	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$	$0,\bar{x},z$	x,x,z	
			$0,x,\bar{z}$	$x,0,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$	
6	g	$m\,m\,2$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	
6	f	$m\,m\,2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$	
6	e	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	d	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
2	c	$6\,m\,m$	$0,0,z$	$0,0,\bar{z}$					
1	b	$6/m\,m\,m$	$0,0,\frac{1}{2}$						
1	a	$6/m\,m\,m$	$0,0,0$						

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{6}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{6}2mm$
$\mathbf{a}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{6}\bar{6}2m$ ($\not{6}\bar{6}m2$, 71)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $\not{6}\bar{6}m2$ (71)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $\not{6}6mm$ (68)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $\not{6}622$ (62)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $\not{6}/m11$ ($\not{6}/m$, 60)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $\not{3}\bar{3}m1$ ($\not{3}\bar{3}1m$, 51)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $\not{3}\bar{3}1m$ (51)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[3] $\not{m}mmm$ ($\not{m}mmm$, 20)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $\not{m}mmm$ ($\not{m}mmm$, 20)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $\not{m}mmm$ ($\not{m}mmm$, 20)	1; 4; 9; 12; 13; 16; 21; 24
IIa	none	
IIb	[2] $\not{6}_3/mmc$ ($\mathbf{c}' = 2\mathbf{c}$) (75); [2] $\not{6}_3/mcm$ ($\mathbf{c}' = 2\mathbf{c}$) ($\not{6}_3/mmc$, 75); [2] $\not{6}/mcc$ ($\mathbf{c}' = 2\mathbf{c}$) (74)	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\not{6}/mmm$ ($\mathbf{c}' = 2\mathbf{c}$) (73)

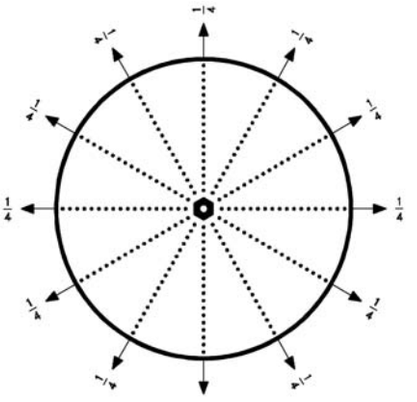
Minimal non-isotypic non-enantiomorphic supergroups

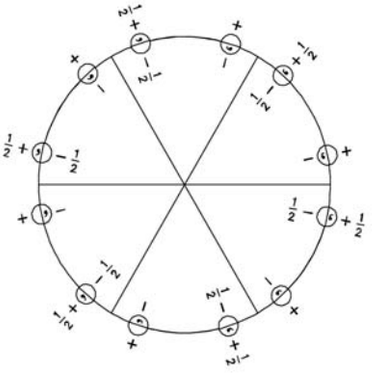
I none

II none

$\not{p}6/mcc$ $6/mmm$ Hexagonal

No. 74 $\not{p}6/m2/c2/c$ Patterson symmetry $\not{p}6/mmm$





Origin at centre $(6/m)$ at $6/mcc$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) 2 $x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) 2 $x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(9) 2 $0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(10) 2 $x,\bar{x},\frac{1}{4}$
$(2_3|0,0,\frac{1}{2})$

(11) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) 2 $2x,x,\frac{1}{4}$
$(2_1|0,0,\frac{1}{2})$

(13) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(14) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(15) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(16) m $x,y,0$
$(m_z|0,0,0)$

(17) $\bar{6}^-$ $0,0,z;\ 0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(18) $\bar{6}^+$ $0,0,z;\ 0,0,0$
$(\bar{6}_z|0,0,0)$

(19) c $x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(20) c $x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(21) c $2x,x,z$
$(m_y|0,0,\frac{1}{2})$

(22) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(23) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(24) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	
			(16) $x,y,\bar{z}$	(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$	
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$	
			(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	
						Special: no extra conditions
12	f	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$
			$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	$\bar{x}+y,y,\frac{1}{2}$	$x,x-y,\frac{1}{2}$
12	e	. . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{1}{4}$	$2x,x,\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$
			$2x,x,\frac{3}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	$2\bar{x},\bar{x},\frac{3}{4}$	$x,2x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$
12	d	. 2 .	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,\bar{x},\frac{1}{4}$	$x,x,\frac{1}{4}$
			$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$
4	c	6 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$		
2	b	$6/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$				
2	a	6 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{2}mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{2}mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{6}\bar{2}c$ ($\not{6}\bar{c}2$, 72)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $\not{6}\bar{c}2$ (72)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $\not{6}cc$ (69)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $\not{6}22$ (62)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $\not{6}/m11$ ($\not{6}/m$, 60)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $\not{3}c1$ ($\not{3}1c$, 52)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $\not{3}1c$ (52)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[3] $\not{m}cc$ ($\not{c}cm$, 21)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $\not{m}cc$ ($\not{c}cm$, 21)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $\not{m}cc$ ($\not{c}cm$, 21)	1; 4; 9; 12; 13; 16; 21; 24
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{6}/mcc$ ($\mathbf{c}'=3\mathbf{c}$) (74)

Minimal non-isotypic non-enantiomorphic supergroups

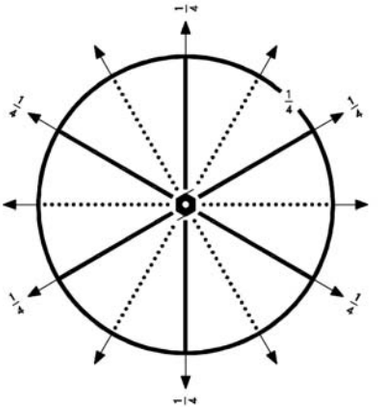
I none

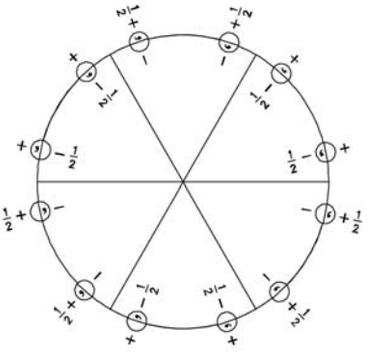
II [2] $\not{6}/mmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (73)

$\not{p}6_3/mmc$ $6/mmm$ Hexagonal

No. 75 $\not{p}6_3/m2/m2/c$ Patterson symmetry $\not{p}6/mmm$

FIRST SETTING





Origin at centre $(\bar{3}m1)$ at $\bar{3}2/mc$

Asymmetric unit $y \le x/2; \quad -x \le y; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2})$ $0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2})$ $0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2})$ $0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) 2 $x,\bar{x},\frac{1}{4}$
$(2_3|0,0,\frac{1}{2})$

(11) 2 $x,2x,\frac{1}{4}$
$(2_2|0,0,\frac{1}{2})$

(12) 2 $2x,x,\frac{1}{4}$
$(2_1|0,0,\frac{1}{2})$

(13) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(14) $\bar{3}^+$ $0,0,z;\ 0,0,0$
$(\bar{3}_z|0,0,0)$

(15) $\bar{3}^-$ $0,0,z;\ 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(16) m $x,y,\frac{1}{4}$
$(m_z|0,0,\frac{1}{2})$

(17) $\bar{6}^-$ $0,0,z;\ 0,0,\frac{1}{4}$
$(\bar{6}_z^{-1}|0,0,\frac{1}{2})$

(18) $\bar{6}^+$ $0,0,z;\ 0,0,\frac{1}{4}$
$(\bar{6}_z|0,0,\frac{1}{2})$

(19) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(20) m $x,2x,z$
$(m_x|0,0,0)$

(21) m $2x,x,z$
$(m_y|0,0,0)$

(22) c x,x,z
$(m_3|0,0,\frac{1}{2})$

(23) c $x,0,z$
$(m_2|0,0,\frac{1}{2})$

(24) c $0,y,z$
$(m_1|0,0,\frac{1}{2})$

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Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	h	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$	
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$	
			(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	
						Special: no extra conditions
12	g	$.m.$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z+\frac{1}{2}$	$2x,x,z+\frac{1}{2}$	$\bar{x},x,z+\frac{1}{2}$
			$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$x,2x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$
12	f	$m..$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$
			$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	$\bar{y},\bar{x},\frac{1}{4}$	$\bar{x}+y,y,\frac{1}{4}$	$x,x-y,\frac{1}{4}$
12	e	$.2.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$
			$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$
6	d	$m\,m\,2$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$
4	c	$3\,m.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$		
2	b	$\bar{6}\,m\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				
2	a	$\bar{3}\,m.$	$0,0,0$	$0,0,\frac{1}{2}$				

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $P2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $P2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $P\bar{6}2c$ ($P\bar{6}c2$, 72)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}m2$ (71)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6_3mc$ (70)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P6_322$ (65)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6_3/m11$ ($P6_3/m$, 61)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}1c$ (52)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[2] $P\bar{3}m1$ ($P\bar{3}1m$, 51)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[3] $Pmmc$ ($Pmcm$, 22)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $Pmmc$ ($Pmcm$, 22)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $Pmmc$ ($Pmcm$, 22)	1; 4; 9; 12; 13; 16; 21; 24
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $P6_3/mmc$ ($\mathbf{c}'=3\mathbf{c}$) (75)

Minimal non-isotypic non-enantiomorphic supergroups

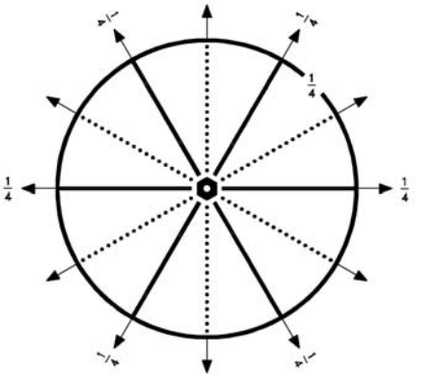
I none

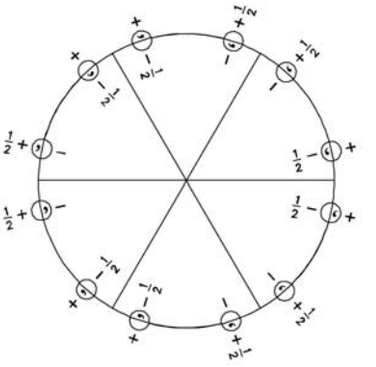
II [2] $P6/mmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (73)

No. 75 $\not{p}6_3/m2/c2/m$

Patterson symmetry $\not{p}6/mmm$

SECOND SETTING





Origin at centre $(\bar{3}1m)$ at $\bar{3}c2/m$

Asymmetric unit $0 \le x; \quad 0 \le y; \quad 0 \le z \le \frac{1}{4}; \quad y \le x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $3^+ \; 0,0,z$
$(3_z|0,0,0)$

(3) $3^- \; 0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $2(\frac{1}{2}) \; 0,0,z$
$(2_z|0,0,\frac{1}{2})$

(5) $6^-(\frac{1}{2}) \; 0,0,z$
$(6_z^{-1}|0,0,\frac{1}{2})$

(6) $6^+(\frac{1}{2}) \; 0,0,z$
$(6_z|0,0,\frac{1}{2})$

(7) $2 \; x,x,\frac{1}{4}$
$(2_{xy}|0,0,\frac{1}{2})$

(8) $2 \; x,0,\frac{1}{4}$
$(2_x|0,0,\frac{1}{2})$

(9) $2 \; 0,y,\frac{1}{4}$
$(2_y|0,0,\frac{1}{2})$

(10) $2 \; x,\bar{x},0$
$(2_3|0,0,0)$

(11) $2 \; x,2x,0$
$(2_2|0,0,0)$

(12) $2 \; 2x,x,0$
$(2_1|0,0,0)$

(13) $\bar{1} \; 0,0,0$
$(\bar{1}|0,0,0)$

(14) $\bar{3}^+ \; 0,0,z; \; 0,0,0$
$(\bar{3}_z|0,0,0)$

(15) $\bar{3}^- \; 0,0,z; \; 0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(16) $m \; x,y,\frac{1}{4}$
$(m_z|0,0,\frac{1}{2})$

(17) $\bar{6}^- \; 0,0,z; \; 0,0,\frac{1}{4}$
$(\bar{6}_z^{-1}|0,0,\frac{1}{2})$

(18) $\bar{6}^+ \; 0,0,z; \; 0,0,\frac{1}{4}$
$(\bar{6}_z|0,0,\frac{1}{2})$

(19) $c \; x,\bar{x},z$
$(m_{xy}|0,0,\frac{1}{2})$

(20) $c \; x,2x,z$
$(m_x|0,0,\frac{1}{2})$

(21) $c \; 2x,x,z$
$(m_y|0,0,\frac{1}{2})$

(22) $m \; x,x,z$
$(m_3|0,0,0)$

(23) $m \; x,0,z$
$(m_2|0,0,0)$

(24) $m \; 0,y,z$
$(m_1|0,0,0)$

Generators selected (1); $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	h	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	l : $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$	
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$	
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
12	g	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	$x,x,z+\frac{1}{2}$
			$0,x,\bar{z}+\frac{1}{2}$	$x,0,\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$
12	f	m . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$
			$y,x,\frac{1}{4}$	$x-y,\bar{y},\frac{1}{4}$	$\bar{x},\bar{x}+y,\frac{1}{4}$	$\bar{y},\bar{x},\frac{3}{4}$	$\bar{x}+y,y,\frac{3}{4}$	$x,x-y,\frac{3}{4}$
12	e	. . 2	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$
			$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$
6	d	$m\,2\,m$	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$
4	c	$3\,.\,m$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$		
2	b	$\bar{3}\,.\,m$	$0,0,0$	$0,0,\frac{1}{2}$				
2	a	$\bar{6}\,2\,m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$				

Symmetry of special projections

Along [001] $6mm$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $\not{p}2mg$
$\mathbf{a}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	[2] $\not{p}\bar{6}c2$ (72)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $\not{p}\bar{6}2m$ ($\not{p}\bar{6}m2$, 71)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $\not{p}6_3cm$ ($\not{p}6_3mc$, 70)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $\not{p}6_322$ (65)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $\not{p}6_3/m11$ ($\not{p}6_3/m$, 61)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $\not{p}\bar{3}c1$ ($\not{p}\bar{3}1c$, 52)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $\not{p}\bar{3}1m$ (51)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[3] $\not{p}mcm$ ($\not{p}mcm$, 22)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $\not{p}mcm$ ($\not{p}mcm$, 22)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $\not{p}mcm$ ($\not{p}mcm$, 22)	1; 4; 9; 12; 13; 16; 21; 24
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\not{p}6_3/mcm$ ($\mathbf{c}'=3\mathbf{c}$) ($\not{p}6_3/mmc$, 75)

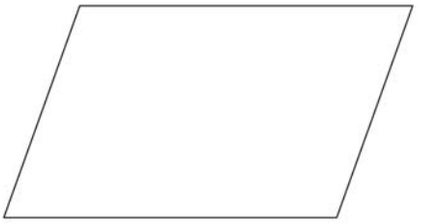
Minimal non-isotypic non-enantiomorphic supergroups

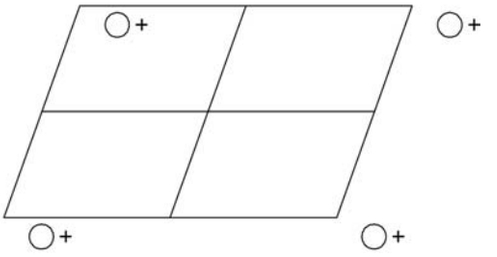
I none

II [2] $\not{p}6/mmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (73)

$p\,1$ 1 Triclinic/Oblique

No. 1 $p\,1$ Patterson symmetry $p\,\bar{1}$





Origin arbitrary

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1$

Symmetry operations

(1) 1
$(1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
1 a 1	(1) x,y,z	no conditions

Symmetry of special projections

Along [001] $p\,1$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not{p}\,1\,1\,1$
$\mathbf{a}' = \mathbf{b}_p$
Origin at $x,0,0$

Along [010] $\not{p}\,1\,1\,1$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I none

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $p\,1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (1)

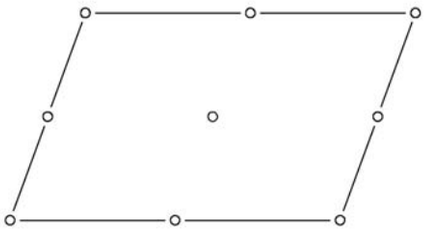
Minimal non-isotypic supergroups

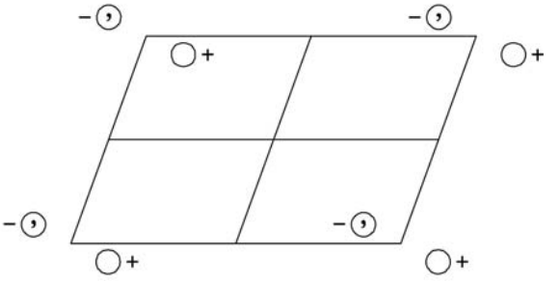
I [2] $p\,\bar{1}$ (2); [2] $p\,1\,1\,2$ (3); [2] $p\,1\,1\,m$ (4); [2] $p\,1\,1\,a$ (5); [2] $p\,2\,1\,1$ (8); [2] $p\,2_1\,1\,1$ (9); [2] $c\,2\,1\,1$ (10); [2] $p\,m\,1\,1$ (11); [2] $p\,b\,1\,1$ (12); [2] $c\,m\,1\,1$ (13); [3] $p\,3$ (65)

II none

$p\,\bar{1}$ $\bar{1}$ Triclinic/Oblique

No. 2 $p\,\bar{1}$ Patterson symmetry $p\,\bar{1}$





Origin at $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (1|0,0,0)
(2) $\bar{1}$ 0,0,0 ($\bar{1}$|0,0,0)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$	no conditions
					Special: no extra conditions
1	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$		
1	c	$\bar{1}$	$\frac{1}{2},0,0$		
1	b	$\bar{1}$	$0,\frac{1}{2},0$		
1	a	$\bar{1}$	$0,0,0$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not{p}211$
$\mathbf{a}' = \mathbf{b}_p$
Origin at $x,0,0$

Along [010] $\not{p}211$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p\,1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups of lowest index

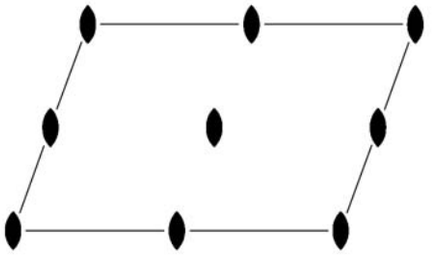
IIc [2] $p\,\bar{1}$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (2)

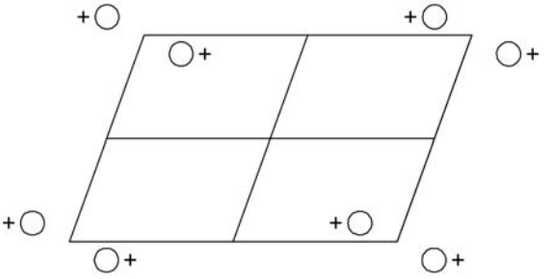
Minimal non-isotypic supergroups

I [2] $p\,1\,1\,2/m$ (6); [2] $p\,1\,1\,2/a$ (7); [2] $p\,2/m\,1\,1$ (14); [2] $p\,2_1/m\,1\,1$ (15); [2] $p\,2/b\,1\,1$ (16); [2] $p\,2_1/b\,1\,1$ (17); [2] $c\,2/m\,1\,1$ (18); [3] $p\,\bar{3}$ (66)
II none

$p\,1\,1\,2$ 2 Monoclinic/Oblique

No. 3 $p\,1\,1\,2$ Patterson symmetry $p\,1\,1\,2/m$





Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$
$(1|0,0,0)$ $(2_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
2	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	General: no conditions
					Special: no extra conditions
1	d	2	$\frac{1}{2},\frac{1}{2},z$		
1	c	2	$\frac{1}{2},0,z$		
1	b	2	$0,\frac{1}{2},z$		
1	a	2	$0,0,z$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not\perp 1m1$
$\mathbf{a}' = \mathbf{b}_p$
Origin at $x,0,0$

Along [010] $\not\perp 1m1$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1(1)2$ 1

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $p112$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (3)

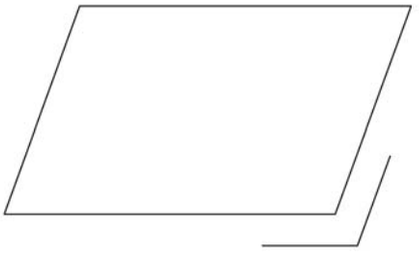
Minimal non-isotypic supergroups

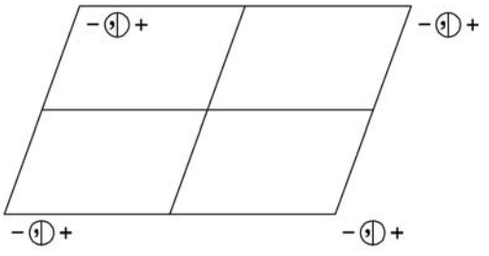
I [2] $p112/m$ (6); [2] $p112/a$ (7); [2] $p222$ (19); [2] $p2_122$ (20); [2] $p2_12_12$ (21); [2] $c222$ (22); [2] $pmm2$ (23); [2] $pma2$ (24); [2] $pba2$ (25); [2] $cmm2$ (26); [2] $p4$ (49); [2] $p\bar{4}$ (50); [3] $p6$ (73)

II none

$p\,1\,1\,m$ m Monoclinic/Oblique

No. 4 $p\,1\,1\,m$ Patterson symmetry $p\,1\,1\,2/m$





Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2 b 1		(1) x,y,z	(2) $x,y,\bar{z}$	no conditions
				Special: no extra conditions
1 a m		$x,y,0$		

Symmetry of special projections

Along [001] $p\,1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}\,1\,1\,m$
$\mathbf{a}' = \mathbf{b}_p$
Origin at $x,0,0$

Along [010] $\not{m}\,1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p\,1\,(1)$ 1

IIa none

IIb [2] $p\,1\,1\,a$ ($\mathbf{a}' = 2\mathbf{a}$) (5); [2] $p\,1\,1\,b$ ($\mathbf{b}' = 2\mathbf{b}$) ($p\,1\,1\,a$, 5); [2] $c\,1\,1\,a$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p\,1\,1\,a$, 5)

Maximal isotypic subgroups of lowest index

IIc [2] $p\,1\,1\,m$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (4)

Minimal non-isotypic supergroups

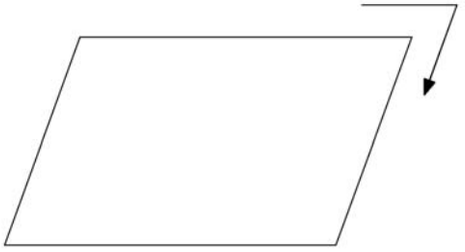
I [2] $p\,1\,1\,2/m$ (6); [2] $p\,m\,2\,m$ (27); [2] $p\,b\,2_1\,m$ (29); [2] $c\,m\,2\,m$ (35); [3] $p\bar{6}$ (74)

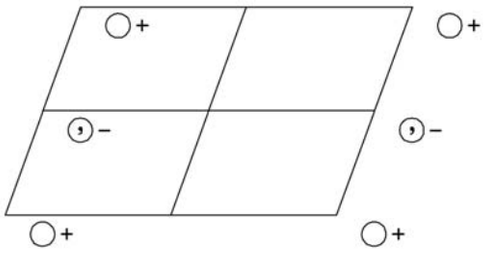
II none

$p\,1\,1\,a$ m Monoclinic/Oblique

No. 5 $p\,1\,1\,a$ Patterson symmetry $p\,1\,1\,2/m$

CELL CHOICE 1





Origin on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 (2) a $x,y,0$
$(1|0,0,0)$ $(m_z|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $x+\frac{1}{2},y,\bar{z}$	hk: $h=2n$ $h0$: $h=2n$

Symmetry of special projections

Along [001] $p\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,m$
$\mathbf{a}'=\mathbf{b}_p$
Origin at $x,0,0$

Along [010] $p\,1\,1\,g$
$\mathbf{a}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p\,1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups of lowest index

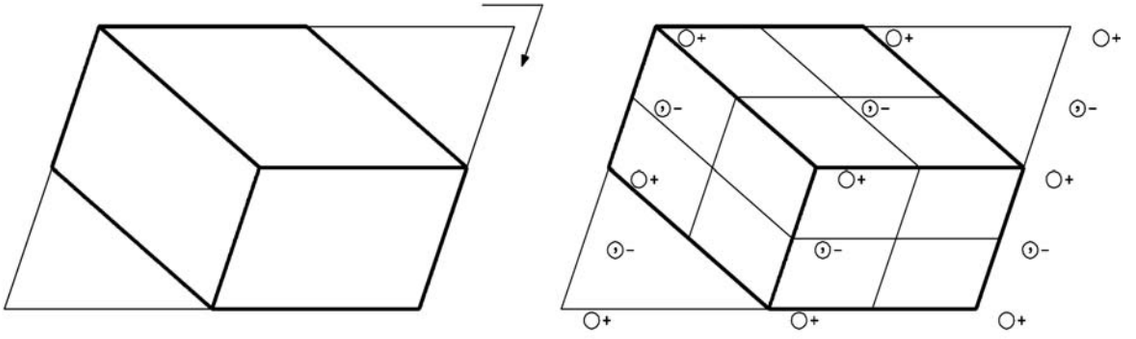
IIc [2] $p\,1\,1\,a$ ($\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=2\mathbf{b}$) (5)

Minimal non-isotypic supergroups

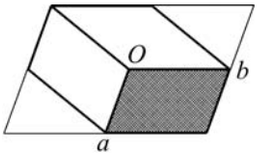
I [2] $p\,1\,1\,2/a$ (7); [2] $pm2_1b$ (28); [2] $pb2b$ (30); [2] $pm2a$ (31); [2] $pm2_1n$ (32); [2] $pb2_1a$ (33); [2] $pb2n$ (34); [2] $cm2e$ (36)
II [2] $p\,1\,1\,m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (4)

No. 5

DIFFERENT CELL CHOICES



p 1 1 *a*



CELL CHOICE 1

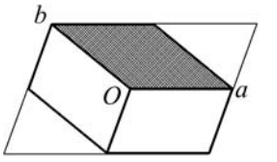
Origin on glide plane *a*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	hk : $h=2n$ $h0$: $h=2n$



p 1 1 *n*

CELL CHOICE 2

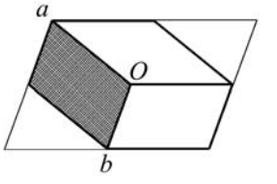
Origin on glide plane *n*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	hk : $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$



p 1 1 *b*

CELL CHOICE 3

Origin on glide plane *b*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z$

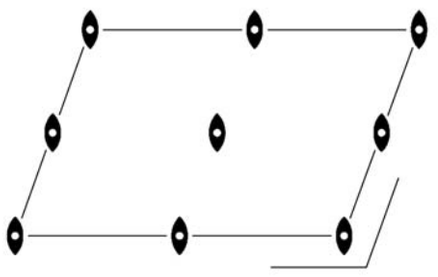
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

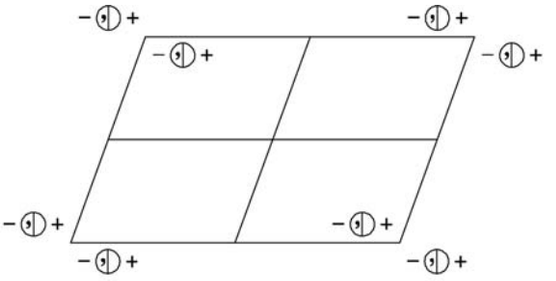
Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x,y+\frac{1}{2},\bar{z}$	hk : $k=2n$ $0k$: $k=2n$

$p\,1\,1\,2/m$ $2/m$ Monoclinic/Oblique

No. 6 $p\,1\,1\,2/m$ Patterson symmetry $p\,1\,1\,2/m$





Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 2 $0,0,z$ $(2_z|0,0,0)$

(3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(4) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	General: no conditions
2	i	m	$x,y,0$	$\bar{x},\bar{y},0$			Special: no extra conditions
2	h	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	g	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	f	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	e	2	$0,0,z$	$0,0,\bar{z}$			
1	d	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	c	$2/m$	$0,\frac{1}{2},0$				
1	b	$2/m$	$\frac{1}{2},0,0$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{b}_p$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p\,1\,1\,m$ (4) 1; 4
[2] $p\,1\,1\,2$ (3) 1; 2
[2] $p\,\bar{1}$ (2) 1; 3

IIa none

IIb [2] $p\,1\,1\,2/a$ ($\mathbf{a}' = 2\mathbf{a}$) (7); [2] $p\,1\,1\,2/b$ ($\mathbf{b}' = 2\mathbf{b}$) ($p\,1\,1\,2/a$, 7); [2] $c\,1\,1\,2/b$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p\,1\,1\,2/a$, 7)

Maximal isotypic subgroups of lowest index

IIc [2] $p\,1\,1\,2/m$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) (6)

Minimal non-isotypic supergroups

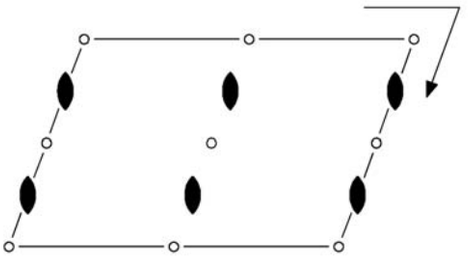
I [2] $pmmm$ (37); [2] $pmam$ (40); [2] $pbam$ (44); [2] $cmmm$ (47); [2] $p\,4/m$ (51); [3] $p\,6/m$ (75)

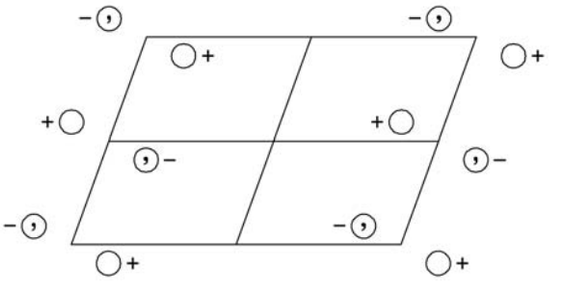
II none

$p\,1\,1\,2/a$ $2/m$ Monoclinic/Oblique

No. 7 $p\,1\,1\,2/a$ Patterson symmetry $p\,1\,1\,2/m$

CELL CHOICE 1





Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1 (1|0,0,0)
(2) 2 $\frac{1}{4},0,z$ $(2_z|\frac{1}{2},0,0)$
(3) $\bar{1}$ 0,0,0 $(\bar{1}|0,0,0)$
(4) a $x,y,0$ $(m_z|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hk : $h=2n$ $h0$: $h=2n$
							Special: no extra conditions
2	d	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			
2	c	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}_p$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p\,1\,1\,a$ (5) 1; 4
[2] $p\,1\,1\,2$ (3) 1; 2
[2] $p\,\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $p\,1\,1\,2/a$ ($\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=2\mathbf{b}$) (7)

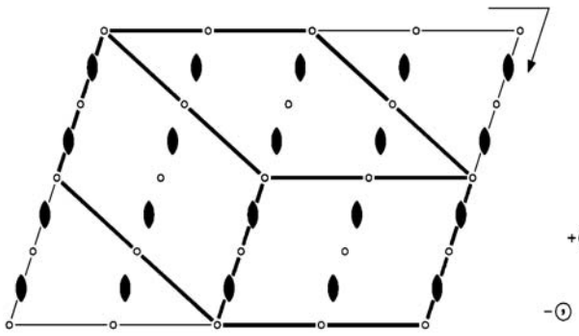
Minimal non-isotypic supergroups

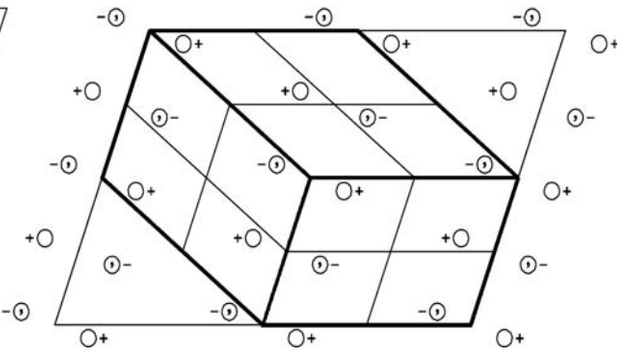
I [2] $pmaa$ (38); [2] $pban$ (39); [2] $pmma$ (41); [2] $pman$ (42); [2] $pbaa$ (43); [2] $pbma$ (45); [2] $pmmn$ (46); [2] $cmme$ (48); [2] $p4/n$ (52)

II [2] $p\,1\,1\,2/m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (6)

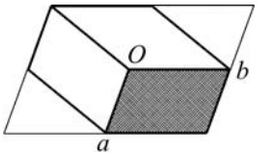
No. 7

DIFFERENT CELL CHOICES





$p\,1\,1\,2/a$



CELL CHOICE 1

Origin at $\bar{1}$ on glide plane a

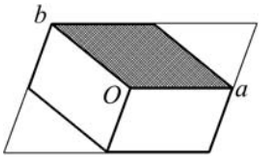
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hk: $h=2n$ $h0$: $h=2n$
							Special: no extra conditions
2	d	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			
2	c	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			

$p112/n$



CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

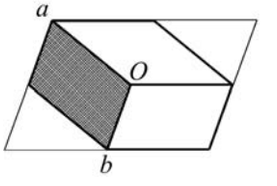
Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	hk : $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: no extra conditions
2	d	2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			
2	c	2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$			
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			

$p112/b$



CELL CHOICE 3

Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

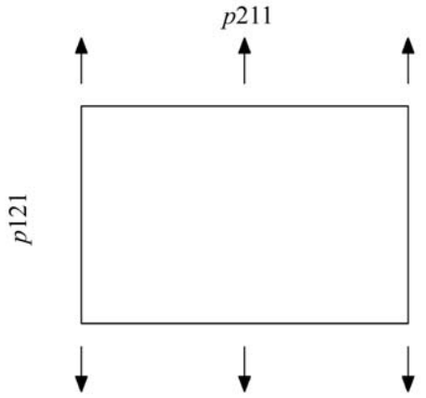
Positions

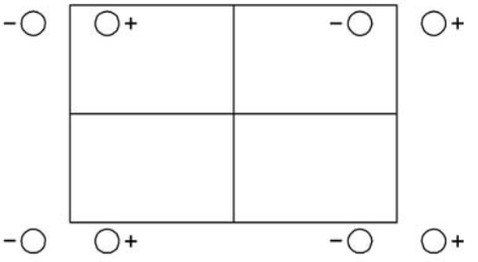
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}$	hk : $k=2n$ $0k$: $k=2n$
							Special: no extra conditions
2	d	2	$\frac{1}{2},\frac{3}{4},z$	$\frac{1}{2},\frac{1}{4},\bar{z}$			
2	c	2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$			
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			

$p211$ 2 Monoclinic/Rectangular

No. 8 $p211$

Patterson symmetry $p2/m11$





Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 2 $x,0,0$ (2_x|0,0,0)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	no conditions
					Special: no extra conditions
1	b	2	$x,\frac{1}{2},0$		
1	a	2	$x,0,0$		

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = -\mathbf{a}$
Origin at $0,0,z$

Along [100] $p211$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1$ (1) 1

IIa none

IIb [2] $c211$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (10); [2] $p2_1 11$ ($\mathbf{a}' = 2\mathbf{a}$) (9)

Maximal isotypic subgroups of lowest index

IIc [2] $p211$ ($\mathbf{a}' = 2\mathbf{a}$) (8); [2] $p211$ ($\mathbf{b}' = 2\mathbf{b}$) (8)

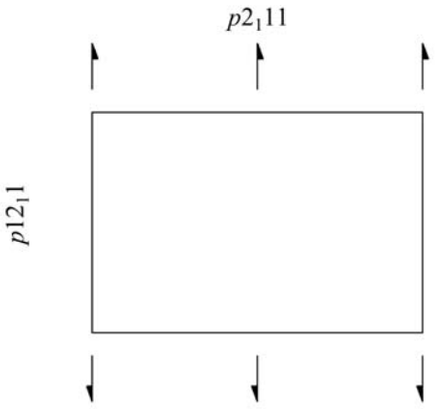
Minimal non-isotypic supergroups

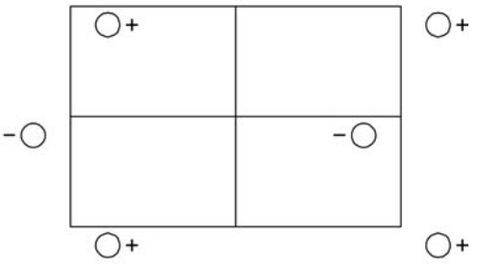
I [2] $p2/m11$ (14); [2] $p2/b11$ (16); [2] $p222$ (19); [2] $p2_122$ (20); [2] $pm2m$ (27); [2] $pb2b$ (30); [2] $pm2a$ (31); [2] $pb2n$ (34)

II [2] $c211$ (10)

$p2_111$ 2 Monoclinic/Rectangular

No. 9 $p2_111$ Patterson symmetry $p2/m11$





Origin on 2_1

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (1|0,0,0)
(2) $2(\frac{1}{2},0,0)$ $x,0,0$ $(2_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $x+\frac{1}{2},\bar{y},\bar{z}$	$h0\colon\ h=2n$

Symmetry of special projections

Along [001] $p1g1$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=-\mathbf{a}$
Origin at $0,0,z$

Along [100] $\not p211$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p11g$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $p2_111$ ($\mathbf{b}'=2\mathbf{b}$) (9); [3] $p2_111$ ($\mathbf{a}'=3\mathbf{a}$) (9)

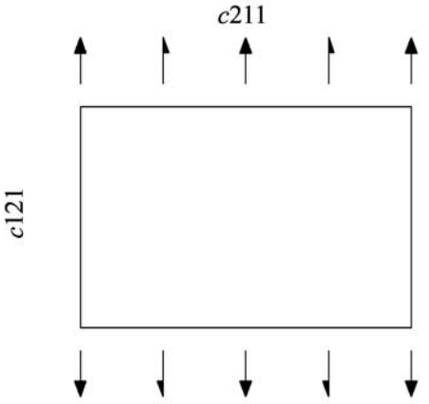
Minimal non-isotypic supergroups

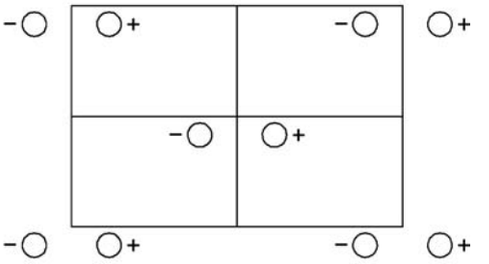
I [2] $p2_1/m11$ (15); [2] $p2_1/b11$ (17); [2] $p2_122$ (20); [2] $p2_12_12$ (21); [2] $pm2_1b$ (28); [2] $pb2_1m$ (29); [2] $pm2_1n$ (32); [2] $pb2_1a$ (33)

II [2] $c211$ (10); [2] $p211$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (8)

$c211$ 2 Monoclinic/Rectangular

No. 10 $c211$ Patterson symmetry $c2/m11$





Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $(1|0,0,0)$ (2) 2 $x,0,0$ $(2_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1|\frac{1}{2},\frac{1}{2},0)$ (2) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
			General:
4 b 1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
			Special: no extra conditions
2 a 2	$x,0,0$		

Symmetry of special projections

Along [001] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = -\mathbf{a}$
Origin at $0,0,z$

Along [100] $\not{c}\,2\,1\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}\,1\,1\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $c\,1$ ($p\,1$, 1) 1+

IIa [2] $p\,2_1\,1\,1$ (9) 1; $2+(\frac{1}{2},\frac{1}{2},0)$
[2] $p\,2\,1\,1$ (8) 1; 2

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $c\,2\,1\,1$ ($\mathbf{a}' = 3\mathbf{a}$) (10)

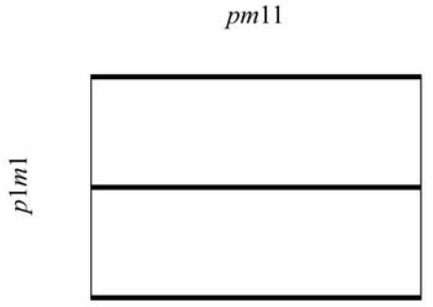
Minimal non-isotypic supergroups

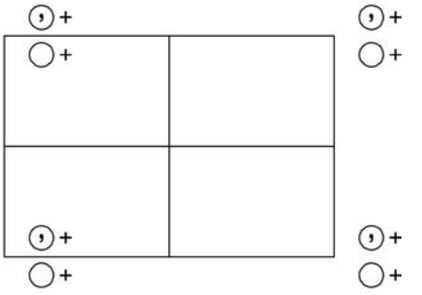
I [2] $c\,2/m\,1\,1$ (18); [2] $c\,2\,2\,2$ (22); [2] $c\,m\,2\,m$ (35); [2] $c\,m\,2\,e$ (36); [3] $p\,3\,1\,2$ (67); [3] $p\,3\,2\,1$ (68)

II [2] $p\,2\,1\,1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (8)

$pm11$ m Monoclinic/Rectangular

No. 11 $pm11$ Patterson symmetry $p2/m11$





Origin on mirror plane m

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$
(2) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $\bar{x},y,z$	no conditions
					Special: no extra conditions
1	b	m	$\frac{1}{2},y,z$		
1	a	m	$0,y,z$		

Symmetry of special projections

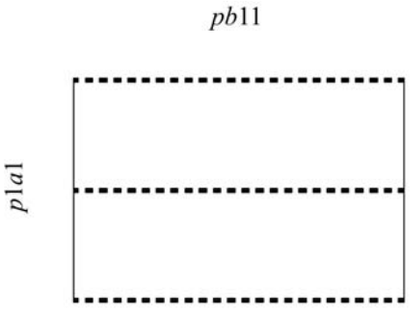
Along [001] $p1m1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

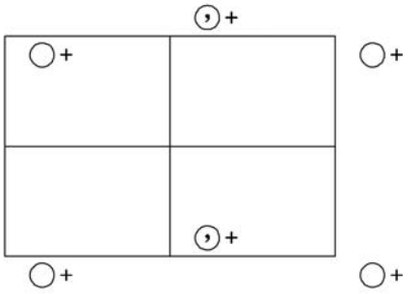
Along [100] $\not\!\!\!

$pb11$ m Monoclinic/Rectangular

No. 12 $pb11$

Patterson symmetry $p2/m11$





Origin on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) b $0,y,z$ $(m_x|0,\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},z$	$0k:\ k=2n$

Symmetry of special projections

Along [001] $p1g1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not{m}11$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{m}1m1$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1$ (1) 1

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [2] $pb11$ ($\mathbf{a}'=2\mathbf{a}$) (12)

Minimal non-isotypic supergroups

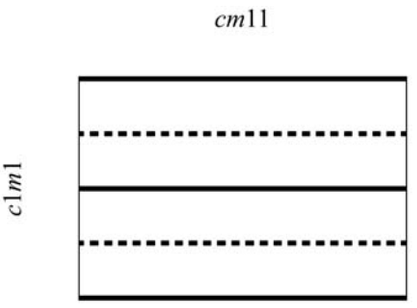
I [2] $p2/b11$ (16); [2] $p2_1/b11$ (17); [2] $pma2$ (24); [2] $pba2$ (25); [2] $pb2_1m$ (29); [2] $pb2b$ (30); [2] $pb2_1a$ (33); [2] $pb2n$ (34)

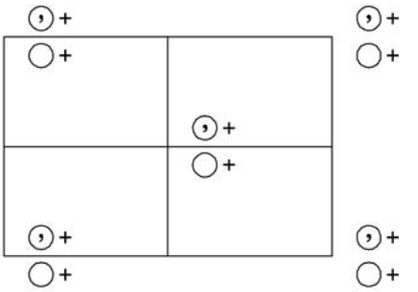
II [2] $cm11$ (13); [2] $pm11$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (11)

International Tables for Crystallography (2010). Vol. E, Layer group 13, pp. 250–251.

$cm11$ m Monoclinic/Rectangular

No. 13 $cm11$ Patterson symmetry $c2/m11$





Origin on mirror plane m

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $(1|0,0,0)$

(2) m $0,y,z$ $(m_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1|\frac{1}{2},\frac{1}{2},0)$

(2) b $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
	$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4 b 1	(1) x,y,z	(2) $\bar{x},y,z$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
			Special: no extra conditions
2 a m	$0,y,z$		

Symmetry of special projections

Along [001] $c\,1\,m\,1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not{m}\,1\,1\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{m}\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $c\,1$ ($p\,1$, 1) 1+

IIa [2] $p\,b\,1\,1$ (12) 1; $2+(\frac{1}{2},\frac{1}{2},0)$
[2] $p\,m\,1\,1$ (11) 1; 2

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $c\,m\,1\,1$ ($\mathbf{a}'=3\mathbf{a}$) (13)

Minimal non-isotypic supergroups

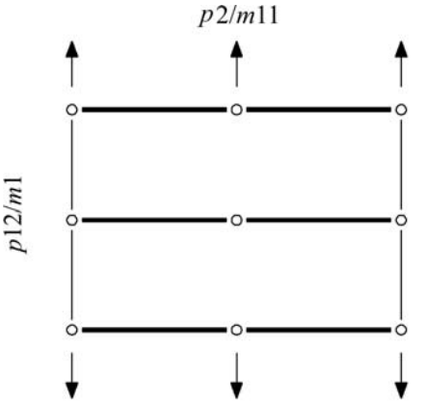
I [2] $c\,2/m\,1\,1$ (18); [2] $c\,m\,m\,2$ (26); [2] $c\,m\,2\,m$ (35); [2] $c\,m\,2\,e$ (36); [3] $p\,3\,m\,1$ (69); [3] $p\,3\,1\,m$ (70)

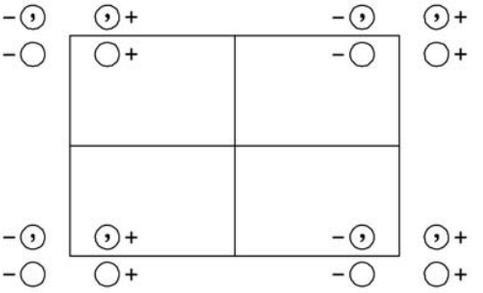
II [2] $p\,m\,1\,1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (11)

$p2/m11$ $2/m$ Monoclinic/Rectangular

No. 14 $p2/m11$

Patterson symmetry $p2/m11$





Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $x,0,0$ $(2_x|0,0,0)$ (3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$ (4) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x},y,z$	General: no conditions
2	h	m	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},\bar{z}$			Special: no extra conditions
2	g	m	$0,y,z$	$0,\bar{y},\bar{z}$			
2	f	2	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	e	2	$x,0,0$	$\bar{x},0,0$			
1	d	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	c	$2/m$	$0,\frac{1}{2},0$				
1	b	$2/m$	$\frac{1}{2},0,0$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not\!p211$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not\!p2mm$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm11$ (11) 1; 4
[2] $p211$ (8) 1; 2
[2] $p\bar{1}$ (2) 1; 3

IIa none

IIb [2] $c2/m11$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (18); [2] $p2/b11$ ($\mathbf{b}' = 2\mathbf{b}$) (16); [2] $p2_1/m11$ ($\mathbf{a}' = 2\mathbf{a}$) (15)

Maximal isotypic subgroups of lowest index

IIc [2] $p2/m11$ ($\mathbf{a}' = 2\mathbf{a}$) (14); [2] $p2/m11$ ($\mathbf{b}' = 2\mathbf{b}$) (14)

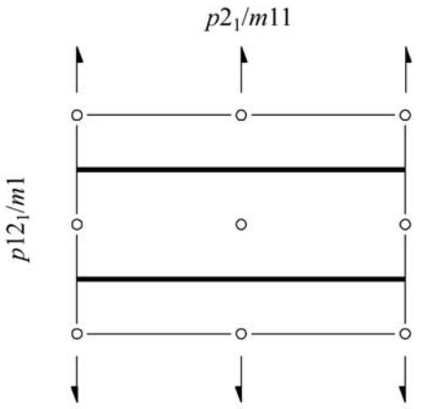
Minimal non-isotypic supergroups

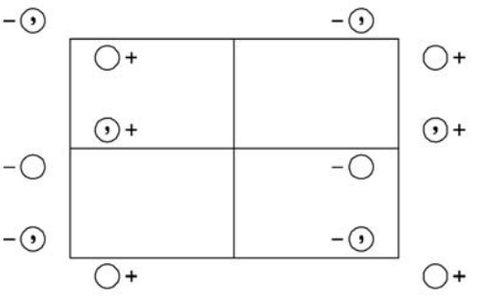
I [2] $pmmm$ (37); [2] $pmaa$ (38); [2] $pmma$ (41); [2] $pman$ (42)

II [2] $c2/m11$ (18)

$p2_1/m11$ $2/m$ Monoclinic/Rectangular

No. 15 $p2_1/m11$ Patterson symmetry $p2/m11$





Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$
(2) $2(\frac{1}{2},0,0)$ $x,0,0$ $(2_x|\frac{1}{2},0,0)$
(3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$
(4) m $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x}+\frac{1}{2},y,z$	$h0$: $h=2n$
							Special: as above, plus
2	c	m	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},\bar{z}$			no extra conditions
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hk : $h=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hk : $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not p211$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm11$ (11) 1; 4
[2] $p2_111$ (9) 1; 2
[2] $p\bar{1}$ (2) 1; 3

IIa none

IIb [2] $p2_1/b11$ ($\mathbf{b}'=2\mathbf{b}$) (17)

Maximal isotypic subgroups of lowest index

IIc [2] $p2_1/m11$ ($\mathbf{b}'=2\mathbf{b}$) (15); [3] $p2_1/m11$ ($\mathbf{a}'=3\mathbf{a}$) (15)

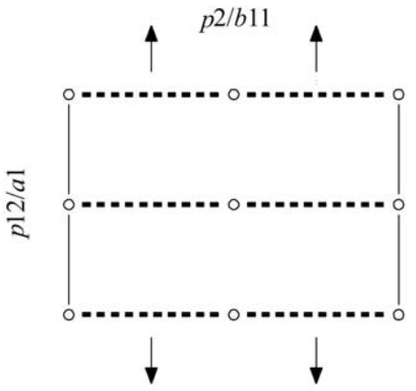
Minimal non-isotypic supergroups

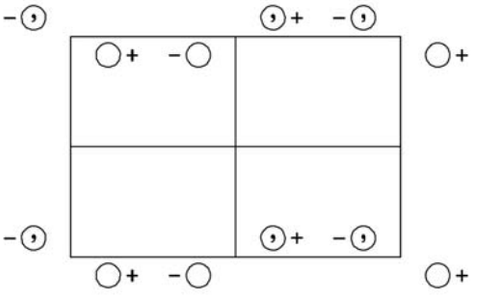
I [2] $pmam$ (40); [2] $pmma$ (41); [2] $pbma$ (45); [2] $pmmn$ (46)

II [2] $c2/m11$ (18); [2] $p2/m11$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (14)

$p2/b11$ $2/m$ Monoclinic/Rectangular

No. 16 $p2/b11$ Patterson symmetry $p2/m11$





Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 2 $x,\frac{1}{4},0$ $(2_x|0,\frac{1}{2},0)$

(3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(4) b $0,y,z$ $(m_x|0,\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $x,\bar{y}+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x},y+\frac{1}{2},z$	$0k:\ k=2n$
							Special: as above, plus
2	c	2	$x,\frac{1}{4},0$	$\bar{x},\frac{3}{4},0$			no extra conditions
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},0$			$hk:\ k=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			$hk:\ k=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=-\mathbf{a}$
Origin at $0,0,z$

Along [100] $p2_111$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb11$ (12) 1; 4
[2] $p2_111$ (8) 1; 2
[2] $p\bar{1}$ (2) 1; 3

IIa none

IIb [2] $p2_1/b11$ ($\mathbf{a}'=2\mathbf{a}$) (17)

Maximal isotypic subgroups of lowest index

IIc [2] $p2/b11$ ($\mathbf{a}'=2\mathbf{a}$) (16)

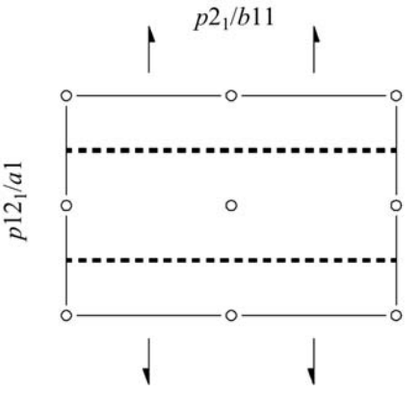
Minimal non-isotypic supergroups

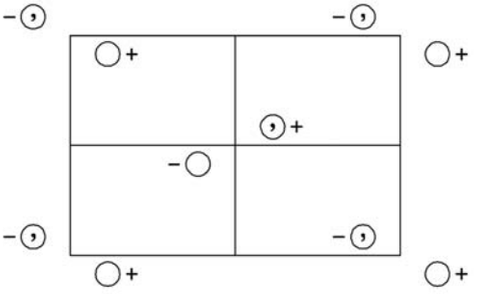
I [2] $pmaa$ (38); [2] $pban$ (39); [2] $pmam$ (40); [2] $pbaa$ (43)

II [2] $c2/m11$ (18); [2] $p2/m11$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (14)

$p2_1/b11$ $2/m$ Monoclinic/Rectangular

No. 17 $p2_1/b11$ Patterson symmetry $p2/m11$





Origin at $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

(3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(4) b $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk : $h+k=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk : $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not p211$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb11$ (12) 1; 4
[2] $p2_111$ (9) 1; 2
[2] $p\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $p2_1/b11$ ($\mathbf{a}'=3\mathbf{a}$) (17)

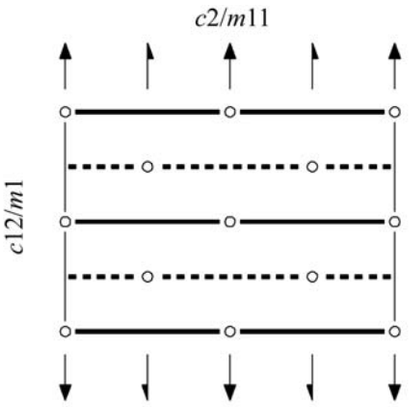
Minimal non-isotypic supergroups

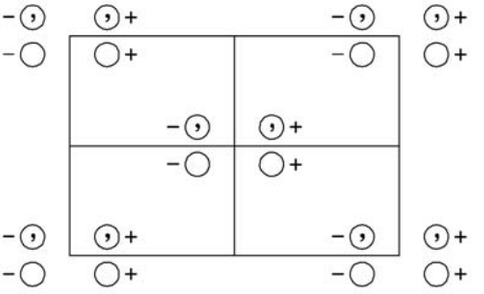
I [2] $pman$ (42); [2] $pbaa$ (43); [2] $pbam$ (44); [2] $pbma$ (45)

II [2] $c2/m11$ (18); [2] $p2_1/m11$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (15); [2] $p2/b11$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (16)

$c2/m11$ $2/m$ Monoclinic/Rectangular

No. 18 $c2/m11$ Patterson symmetry $c2/m11$





Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $(1|0,0,0)$ (2) 2 $x,0,0$ $(2_x|0,0,0)$ (3) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$ (4) m $0,y,z$ $(m_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1|\frac{1}{2},\frac{1}{2},0)$ (2) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$ (3) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ $(\bar{1}|\frac{1}{2},\frac{1}{2},0)$ (4) b $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $\bar{x},y,z$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	e	m	$0,y,z$	$0,\bar{y},\bar{z}$			no extra conditions
4	d	2	$x,0,0$	$\bar{x},0,0$			no extra conditions
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hk: $k=2n$
2	b	$2/m$	$\frac{1}{2},0,0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $\not\!c211$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not\!c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $cm11$ (13) (1; 4)+
[2] $c211$ (10) (1; 2)+
[2] $c\bar{1}$ ($p\bar{1}$, 2) (1; 3)+

IIa
[2] $p2_1/b11$ (17) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $p2/b11$ (16) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $p2_1/m11$ (15) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $p2/m11$ (14) 1; 2; 3; 4

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $c2/m11$ ($\mathbf{a}'=3\mathbf{a}$) (18)

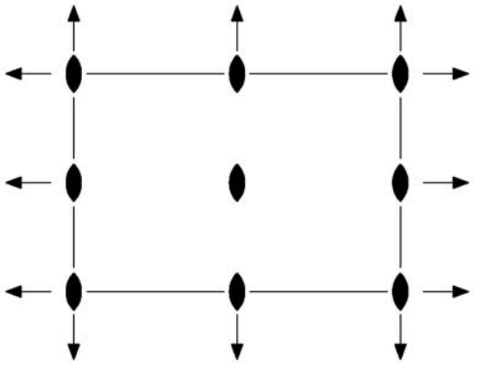
Minimal non-isotypic supergroups

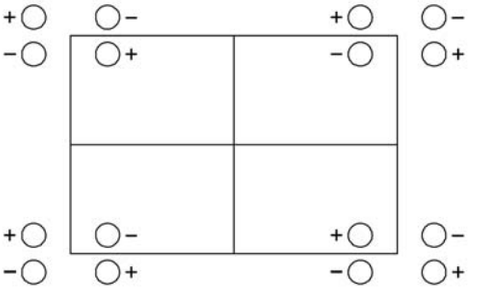
I [2] $cmmm$ (47); [2] $cmme$ (48); [3] $p\bar{3}1m$ (71); [3] $p\bar{3}m1$ (72)

II [2] $p2/m11$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (14)

*p*222 222 Orthorhombic/Rectangular

No. 19 *p*222 Patterson symmetry *pmmm*





Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 2 0,0,*z* (2_z|0,0,0)

(3) 2 0,*y*,0 (2_y|0,0,0)

(4) 2 *x*,0,0 (2_x|0,0,0)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	General: no conditions
							Special: no extra conditions
2	l	. . 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	k	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	j	. . 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	i	. . 2	$0,0,z$	$0,0,\bar{z}$			
2	h	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	g	. 2 .	$0,y,0$	$0,\bar{y},0$			
2	f	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	e	2 . .	$x,0,0$	$\bar{x},0,0$			
1	d	2 2 2	$\frac{1}{2},\frac{1}{2},0$				
1	c	2 2 2	$0,\frac{1}{2},0$				
1	b	2 2 2	$\frac{1}{2},0,0$				
1	a	2 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p121$ ($p211$, 8) 1; 3
[2] $p211$ (8) 1; 4
[2] $p112$ (3) 1; 2

IIa none

IIb [2] $c222$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (22); [2] $p22_12$ ($\mathbf{b}' = 2\mathbf{b}$) ($p2_122$, 20); [2] $p2_122$ ($\mathbf{a}' = 2\mathbf{a}$) (20)

Maximal isotypic subgroups of lowest index

IIc [2] $p222$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (19)

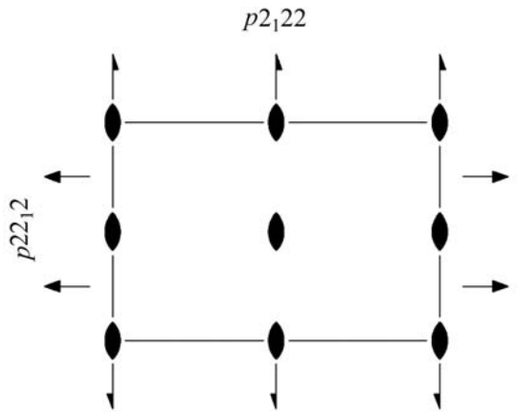
Minimal non-isotypic supergroups

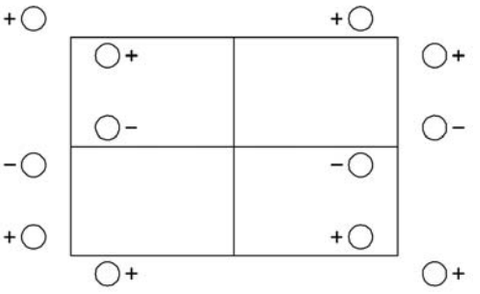
I [2] $pmmm$ (37); [2] $pmaa$ (38); [2] $pban$ (39); [2] $p422$ (53); [2] $p\bar{4}2m$ (57)

II [2] $c222$ (22)

$p2_122$ 222 Orthorhombic/Rectangular

No. 20 $p2_122$ Patterson symmetry $pmmm$





Origin at $2_1 12$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1 (1|0,0,0)
(2) $2(\frac{1}{2},0,0)$ $x,0,0$ $(2_x|\frac{1}{2},0,0)$
(3) 2 $\frac{1}{4},y,0$ $(2_y|\frac{1}{2},0,0)$
(4) 2 $0,0,z$ $(2_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$	(4) $\bar{x},\bar{y},z$	$h0\colon\ h=2n$
							Special: as above, plus
2	c	. 2 .	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$			no extra conditions
2	b	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			$hk\colon\ h=2n$
2	a	. . 2	$0,0,z$	$\frac{1}{2},0,\bar{z}$			$hk\colon\ h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $\frac{1}{4},y,0$

Maximal non-isotypic subgroups

I [2] $p2_11\,1$ (9) 1; 2
[2] $p\,1\,2\,1$ ($p2\,1\,1$, 8) 1; 3
[2] $p\,1\,1\,2$ (3) 1; 4

IIa none

IIb [2] $p2_12_12$ ($\mathbf{b}'=2\mathbf{b}$) (21)

Maximal isotypic subgroups of lowest index

IIc [2] $p2_122$ ($\mathbf{b}'=2\mathbf{b}$) (20); [3] $p2_122$ ($\mathbf{a}'=3\mathbf{a}$) (20)

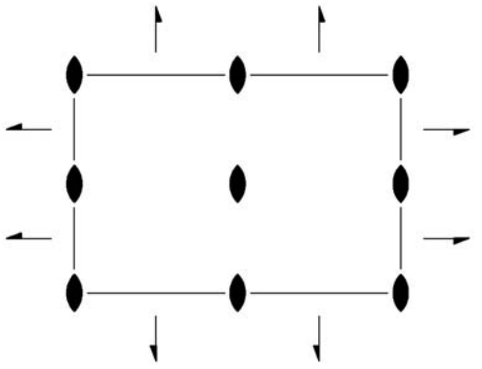
Minimal non-isotypic supergroups

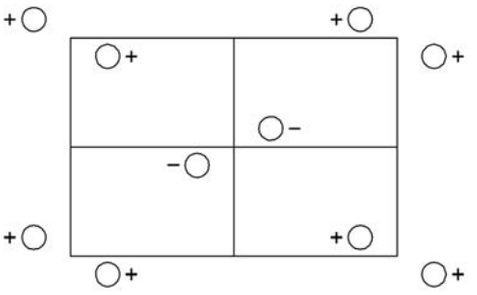
I [2] $pmam$ (40); [2] $pmma$ (41); [2] $pman$ (42); [2] $pbaa$ (43); [2] $pbma$ (45)

II [2] $c222$ (22); [2] $p222$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (19)

$p2_12_12$ 222 Orthorhombic/Rectangular

No. 21 $p2_12_12$ Patterson symmetry $pmmm$





Origin at intersection of 2 with perpendicular plane containing 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 2 0,0,z (2_z|0,0,0)

(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ ($2_y|\frac{1}{2},\frac{1}{2},0$)

(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ ($2_x|\frac{1}{2},\frac{1}{2},0$)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
2	b	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			hk: $h+k=2n$
2	a	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			hk: $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [010] $\not{p}2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $\frac{1}{4},y,0$

Maximal non-isotypic subgroups

I [2] $p12_11$ ($p2_111$, 9) 1; 3
[2] $p2_111$ (9) 1; 4
[2] $p112$ (3) 1; 2

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $p2_12_12$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (21)

Minimal non-isotypic supergroups

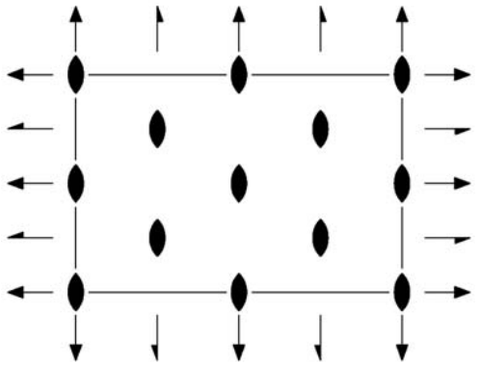
I [2] $pbam$ (44); [2] $pmmn$ (46); [2] $p42_12$ (54); [2] $p\bar{4}2_1m$ (58)

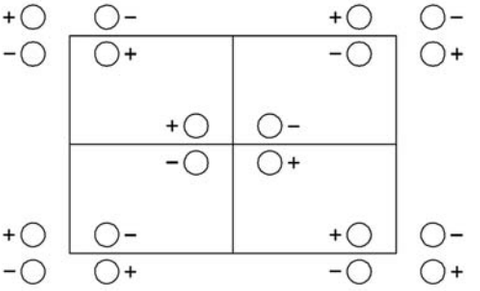
II [2] $c222$ (22); [2] $p22_12$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($p2_122$, 20)

International Tables for Crystallography (2010). Vol. E, Layer group 22, pp. 268–269.

*c*222 222 Orthorhombic/Rectangular

No. 22 *c*222 Patterson symmetry *cmmm*





Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

$(1|0,0,0)$ $(2_z|0,0,0)$ $(2_y|0,0,0)$ $(2_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

$(1|\frac{1}{2},\frac{1}{2},0)$ $(2_z|\frac{1}{2},\frac{1}{2},0)$ $(2_y|\frac{1}{2},\frac{1}{2},0)$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hk: $h+k=2n$ $0k$: $k=2n$ $h0$: $h=2n$
							Special: as above, plus
4	g	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			hk: $h=2n$
4	f	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	e	. . 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	. 2 .	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	c	2 . .	$x,0,0$	$\bar{x},0,0$			no extra conditions
2	b	2 2 2	$0,\frac{1}{2},0$				no extra conditions
2	a	2 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] $c121$ ($c211$, 10)	(1; 3)+
	[2] $c211$ (10)	(1; 4)+
	[2] $c112$ ($p112$, 3)	(1; 2)+
IIa	[2] $p2_12_12$ (21)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $p2_122$ (20)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $p22_12$ ($p2_122$, 20)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $p222$ (19)	1; 2; 3; 4
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $c222$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (22)

Minimal non-isotypic supergroups

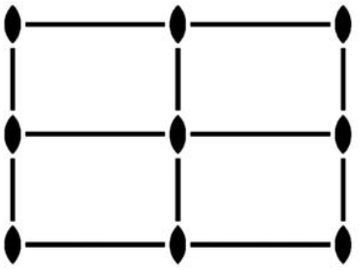
I [2] $cmmm$ (47); [2] $cmme$ (48); [2] $p422$ (53); [2] $p42_12$ (54); [2] $p\bar{4}m2$ (59); [2] $p\bar{4}b2$ (60); [3] $p622$ (76)

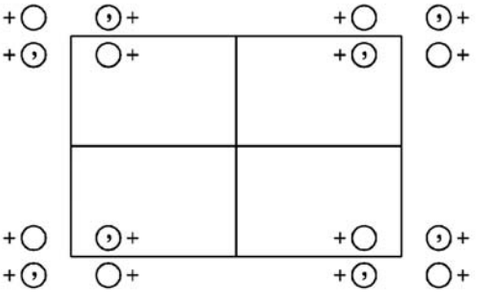
II [2] $p222$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (19)

International Tables for Crystallography (2010). Vol. E, Layer group 23, pp. 270–271.

$pmm2$ $mm2$ Orthorhombic/Rectangular

No. 23 $pmm2$ Patterson symmetry $pmmm$





Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,0,z$ $(2_z|0,0,0)$

(3) $m \quad x,0,z$ $(m_y|0,0,0)$

(4) $m \quad 0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
							Special: no extra conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$m\,m\,2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$m\,m\,2$	$\frac{1}{2},0,z$				
1	b	$m\,m\,2$	$0,\frac{1}{2},z$				
1	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}1m1$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1m1$ ($pm11$, 11) 1; 3
[2] $pm11$ (11) 1; 4
[2] $p112$ (3) 1; 2

IIa none

IIb [2] $cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (26); [2] $pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (24); [2] $pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($pma2$, 24)

Maximal isotypic subgroups of lowest index

IIc [2] $pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (23)

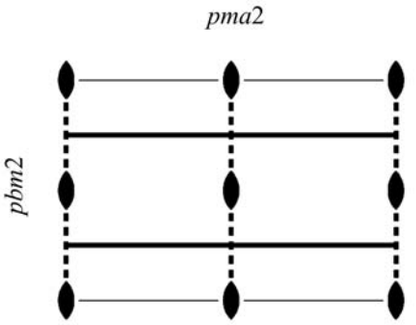
Minimal non-isotypic supergroups

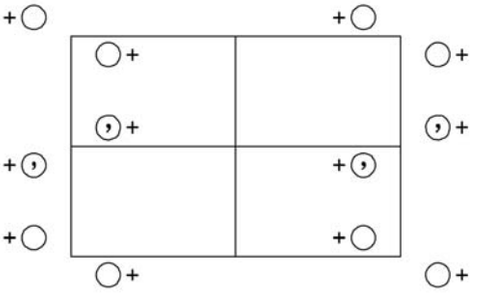
I [2] $pmmm$ (37); [2] $pmma$ (41); [2] $pmmn$ (46); [2] $p4mm$ (55); [2] $p\bar{4}m2$ (59)

II [2] $cmm2$ (26)

$pma2$ $mm2$ Orthorhombic/Rectangular

No. 24 $pma2$ Patterson symmetry $pmmm$





Origin on $1a2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $0,0,z$ $(2_z|0,0,0)$ (3) a $x,0,z$ $(m_y|\frac{1}{2},0,0)$ (4) m $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	$h0$: $h=2n$
							Special: as above, plus
2	c	m . .	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
2	b	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$			hk : $h=2n$
2	a	. . 2	$0,0,z$	$\frac{1}{2},0,z$			hk : $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1a1$ ($pb11$, 12) 1; 3
[2] $pm11$ (11) 1; 4
[2] $p112$ (3) 1; 2

IIa none

IIb [2] $pba2$ ($\mathbf{b}'=2\mathbf{b}$) (25)

Maximal isotypic subgroups of lowest index

IIc [2] $pma2$ ($\mathbf{b}'=2\mathbf{b}$) (24); [3] $pma2$ ($\mathbf{a}'=3\mathbf{a}$) (24)

Minimal non-isotypic supergroups

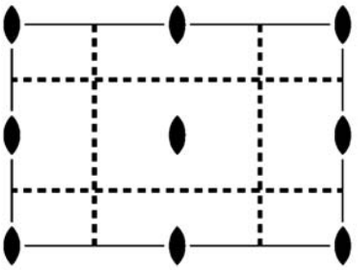
I [2] $pmaa$ (38); [2] $pmam$ (40); [2] $pman$ (42); [2] $pbma$ (45)

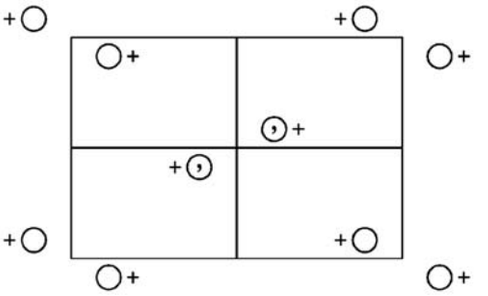
II [2] $cmm2$ (26); [2] $pmm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (23)

$pba2$ $mm2$ Orthorhombic/Rectangular

No. 25 $pba2$

Patterson symmetry $pmmm$





Origin on 112

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1
(1|0,0,0)

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(4) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
2	b	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hk : $h+k=2n$
2	a	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hk : $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p1a1$ ($pb11$, 12) 1; 3
[2] $pb11$ (12) 1; 4
[2] $p112$ (3) 1; 2

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pba2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (25)

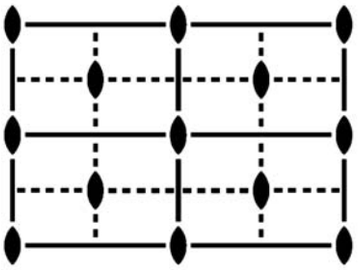
Minimal non-isotypic supergroups

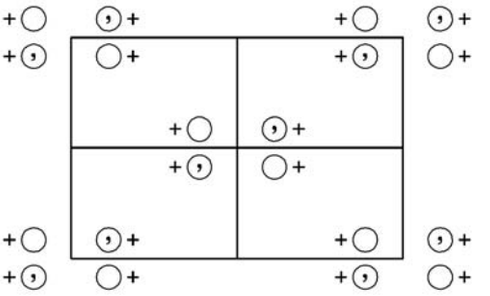
I [2] $pban$ (39); [2] $pbaa$ (43); [2] $pbam$ (44); [2] $p4bm$ (56); [2] $p\bar{4}b2$ (60)

II [2] $cmm2$ (26); [2] $pma2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (24)

$cmm2$ $mm2$ Orthorhombic/Rectangular

No. 26 $cmm2$ Patterson symmetry $cmmm$





Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) m $x,0,z$	(4) m $0,y,z$
$(1\|0,0,0)$	$(2_z\|0,0,0)$	$(m_y\|0,0,0)$	$(m_x\|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) a $x,\frac{1}{4},z$	(4) b $\frac{1}{4},y,z$
$(1\|\frac{1}{2},\frac{1}{2},0)$	$(2_z\|\frac{1}{2},\frac{1}{2},0)$	$(m_y\|\frac{1}{2},\frac{1}{2},0)$	$(m_x\|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hk: $h+k=2n$ $0k$: $k=2n$ $h0$: $h=2n$
							Special: as above, plus
4	e	m . .	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	d	. m .	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	c	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hk: $h=2n$
2	b	$m\,m$ 2	$0,\frac{1}{2},z$				no extra conditions
2	a	$m\,m$ 2	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{c}1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] $c1m1$ ($cm11$, 13)	(1; 3)+
	[2] $cm11$ (13)	(1; 4)+
	[2] $c112$ ($p112$, 3)	(1; 2)+
IIa	[2] $pba2$ (25)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pbm2$ ($pma2$, 24)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pma2$ (24)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pmm2$ (23)	1; 2; 3; 4
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $cmm2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (26)

Minimal non-isotypic supergroups

I [2] $cmmm$ (47); [2] $cmme$ (48); [2] $p4mm$ (55); [2] $p4bm$ (56); [2] $p\bar{4}2m$ (57); [2] $p\bar{4}2_1m$ (58); [3] $p6mm$ (77)

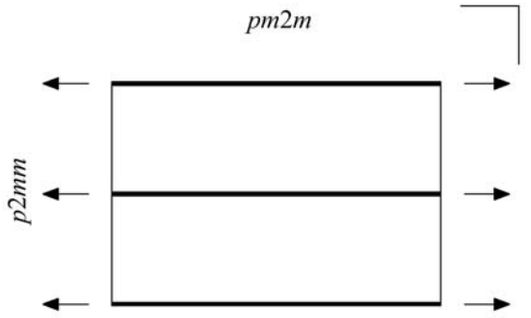
II [2] $pmm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (23)

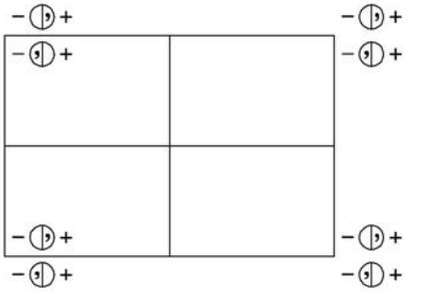
International Tables for Crystallography (2010). Vol. E, Layer group 27, pp. 278–279.

$pm2m$ $m2m$ Orthorhombic/Rectangular

No. 27 $pm2m$

Patterson symmetry $pmmm$





Origin on $m2m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $0,y,0$ $(2_y|0,0,0)$ (3) m $0,y,z$ $(m_x|0,0,0)$ (4) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},y,z$	(4) $x,y,\bar{z}$	General: no conditions
							Special: no extra conditions
2	e	$..m$	$x,y,0$	$\bar{x},y,0$			
2	d	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},y,\bar{z}$			
2	c	$m..$	$0,y,z$	$0,y,\bar{z}$			
1	b	$m2m$	$\frac{1}{2},y,0$				
1	a	$m2m$	$0,y,0$				

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm11$ (11) 1; 3
[2] $p1211$ ($p2111$, 8) 1; 2
[2] $p11m$ (4) 1; 4

IIa none

IIb [2] $cm2e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (36); [2] $cm2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); [2] $pm2a$ ($\mathbf{a}' = 2\mathbf{a}$) (31); [2] $pb2b$ ($\mathbf{b}' = 2\mathbf{b}$) (30); [2] $pb2_1m$ ($\mathbf{b}' = 2\mathbf{b}$) (29); [2] $pm2_1b$ ($\mathbf{b}' = 2\mathbf{b}$) (28)

Maximal isotypic subgroups of lowest index

IIc [2] $pm2m$ ($\mathbf{a}' = 2\mathbf{a}$) (27); [2] $pm2m$ ($\mathbf{b}' = 2\mathbf{b}$) (27)

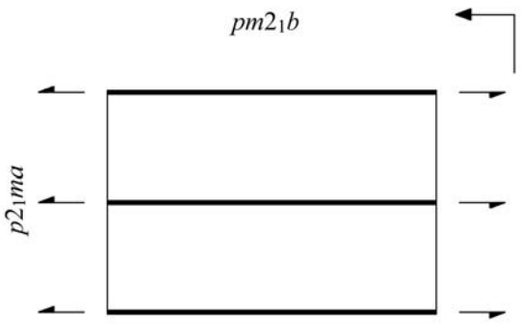
Minimal non-isotypic supergroups

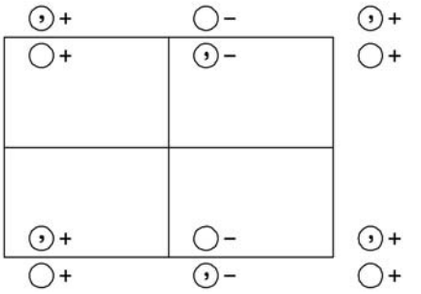
I [2] $pmmm$ (37); [2] $pmam$ (40); [3] $p\bar{6}m2$ (78); [3] $p\bar{6}2m$ (79)

II [2] $cm2m$ (35)

$pm2_1b$ $m2m$ Orthorhombic/Rectangular

No. 28 $pm2_1b$ Patterson symmetry $pmmm$





Origin on $m2_1b$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) $2(0,\frac{1}{2},0)$ $0,y,0$ $(2_y|0,\frac{1}{2},0)$ (3) b $x,y,0$ $(m_z|0,\frac{1}{2},0)$ (4) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	c	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}$	(3) $x,y+\frac{1}{2},\bar{z}$	(4) $\bar{x},y,z$	General:
							hk : $k=2n$
							$0k$: $k=2n$
							Special: no extra conditions
2	b	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},y+\frac{1}{2},\bar{z}$			
2	a	m . .	$0,y,z$	$0,y+\frac{1}{2},\bar{z}$			

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p11g$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm11$ (11) 1; 4
[2] $p12_11$ ($p2_111$, 9) 1; 2
[2] $p11b$ ($p11a$, 5) 1; 3

IIa none

IIb [2] $pm2_1n$ ($\mathbf{a}'=2\mathbf{a}$) (32)

Maximal isotypic subgroups of lowest index

IIc [2] $pm2_1b$ ($\mathbf{a}'=2\mathbf{a}$) (28); [3] $pm2_1b$ ($\mathbf{b}'=3\mathbf{b}$) (28)

Minimal non-isotypic supergroups

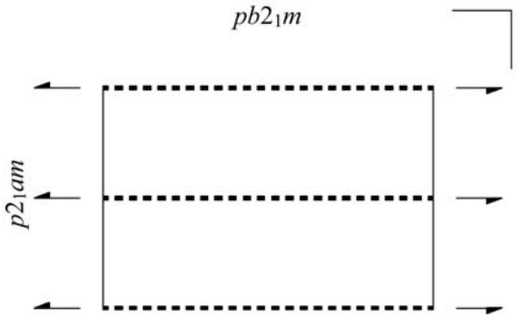
I [2] $pmma$ (41); [2] $pbma$ (45)

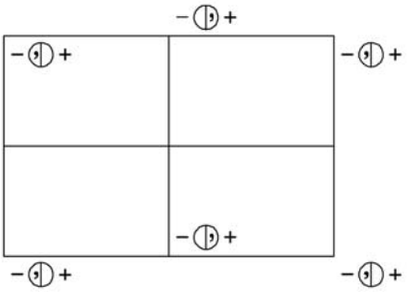
II [2] $cm2m$ (35); [2] $cm2e$ (36); [2] $pm2m$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27)

International Tables for Crystallography (2010). Vol. E, Layer group 29, pp. 282–283.

$pb2_1m$ $m2m$ Orthorhombic/Rectangular

No. 29 $pb2_1m$ Patterson symmetry $pmmm$





Origin on $b2_1m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 (1|0,0,0)
(2) $2(0,\frac{1}{2},0)$ $0,y,0$ $(2_y|0,\frac{1}{2},0)$
(3) b $0,y,z$ $(m_x|0,\frac{1}{2},0)$
(4) m $x,y,0$ $(m_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 b 1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},z$	(4) $x,y,\bar{z}$	$0k:\ k=2n$
					Special: no extra conditions
2 a $..m$	$x,y,0$	$\bar{x},y+\frac{1}{2},0$			

Symmetry of special projections

Along [001] $p1g1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb11$ (12) 1; 3
[2] $p12_11$ ($p2_111$, 9) 1; 2
[2] $p11m$ (4) 1; 4

IIa none

IIb [2] $pb2_1a$ ($\mathbf{a}'=2\mathbf{a}$) (33)

Maximal isotypic subgroups of lowest index

IIc [2] $pb2_1m$ ($\mathbf{a}'=2\mathbf{a}$) (29); [3] $pb2_1m$ ($\mathbf{b}'=3\mathbf{b}$) (29)

Minimal non-isotypic supergroups

I [2] $pmam$ (40); [2] $pbam$ (44)

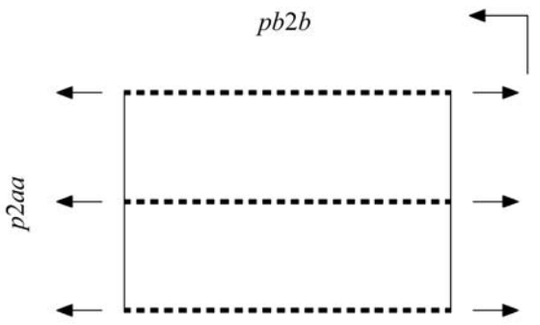
II [2] $pm2m$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27)

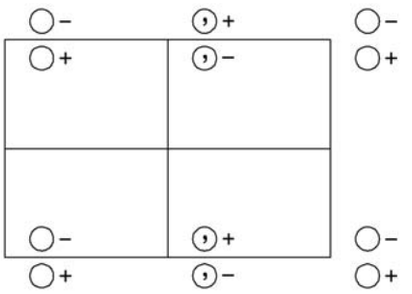
International Tables for Crystallography (2010). Vol. E, Layer group 30, pp. 284–285.

p b 2 b *m 2 m* Orthorhombic/Rectangular

No. 30 *p b 2 b*

Patterson symmetry *p m m m*





Origin on *b*2*b*

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$ (2) 2 $0,y,0$ $(2_y|0,0,0)$ (3) b $x,y,0$ $(m_z|0,\frac{1}{2},0)$ (4) b $0,y,z$ $(m_x|0,\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $x,y+\frac{1}{2},\bar{z}$	(4) $\bar{x},y+\frac{1}{2},z$	General:
							hk : $k=2n$
							$0k$: $k=2n$
							Special: no extra conditions
2	b	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},y+\frac{1}{2},0$			
2	a	. 2 .	$0,y,0$	$0,y+\frac{1}{2},0$			

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb11$ (12) 1; 4
[2] $p121$ ($p211$, 8) 1; 2
[2] $p11b$ ($p11a$, 5) 1; 3

IIa none

IIb [2] $pb2n$ ($\mathbf{a}'=2\mathbf{a}$) (34)

Maximal isotypic subgroups of lowest index

IIc [2] $pb2b$ ($\mathbf{a}'=2\mathbf{a}$) (30); [3] $pb2b$ ($\mathbf{b}'=3\mathbf{b}$) (30)

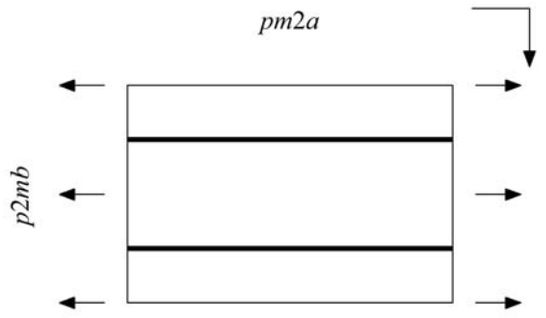
Minimal non-isotypic supergroups

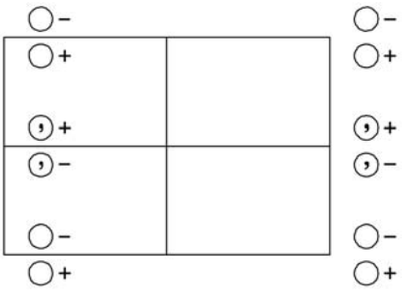
I [2] $pmaa$ (38); [2] $pbaa$ (43)

II [2] $cm2e$ (36); [2] $pm2m$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27)

$pm2a$ $m2m$ Orthorhombic/Rectangular

No. 31 $pm2a$ Patterson symmetry $pmmm$





Origin on 12*a*

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (1|0,0,0)
(2) 2 0,*y*,0 (2_y|0,0,0)
(3) *a* *x*,*y*,0 ($m_z|\frac{1}{2},0,0$)
(4) *m* $\frac{1}{4},y,z$ ($m_x|\frac{1}{2},0,0$)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $x+\frac{1}{2},y,\bar{z}$	(4) $\bar{x}+\frac{1}{2},y,z$	hk : $h=2n$ $h0$: $h=2n$
							Special: no extra conditions
2	b	m . .	$\frac{1}{4},y,z$	$\frac{3}{4},y,\bar{z}$			
2	a	. 2 .	$0,y,0$	$\frac{1}{2},y,0$			

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}11m$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{m}2mg$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm11$ (11) 1; 4
[2] $p121$ ($p211$, 8) 1; 2
[2] $p11a$ (5) 1; 3

IIa none

IIb [2] $pb2n$ ($\mathbf{b}' = 2\mathbf{b}$) (34); [2] $pb2_1a$ ($\mathbf{b}' = 2\mathbf{b}$) (33); [2] $pm2_1n$ ($\mathbf{b}' = 2\mathbf{b}$) (32)

Maximal isotypic subgroups of lowest index

IIc [2] $pm2a$ ($\mathbf{b}' = 2\mathbf{b}$) (31); [3] $pm2a$ ($\mathbf{a}' = 3\mathbf{a}$) (31)

Minimal non-isotypic supergroups

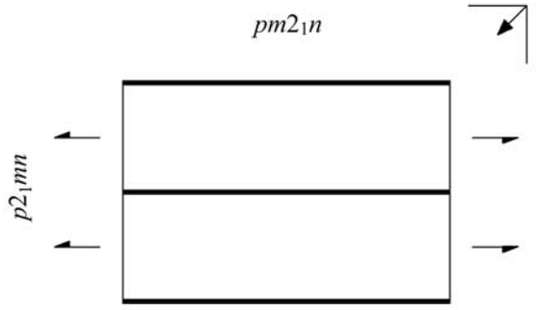
I [2] $pmaa$ (38); [2] $pmma$ (41)

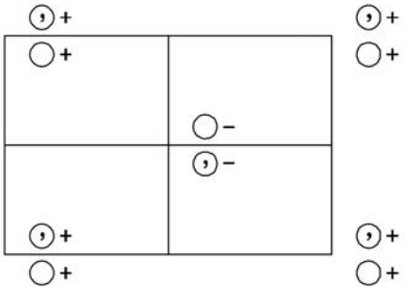
II [2] $cm2e$ (36); [2] $pm2m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (27)

International Tables for Crystallography (2010). Vol. E, Layer group 32, pp. 288–289.

$pm2_1n$ $m2m$ Orthorhombic/Rectangular

No. 32 $pm2_1n$ Patterson symmetry $pmmm$





Origin on $m1n$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ $(2_y|\frac{1}{2},\frac{1}{2},0)$

(3) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$ $(m_z|\frac{1}{2},\frac{1}{2},0)$

(4) m $0,y,z$ $(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $\bar{x},y,z$	General: hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
2 a m . .	$0,y,z$	$\frac{1}{2},y+\frac{1}{2},\bar{z}$			Special: no extra conditions

Symmetry of special projections

Along [001] $c\,1\,m\,1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}\,1\,1\,g$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{m}\,2\,m\,g$
$\mathbf{a}'=\mathbf{a}$
Origin at $\frac{1}{4},y,0$

Maximal non-isotypic subgroups

I [2] $pm\,1\,1$ (11) 1; 4
[2] $p\,1\,2_1\,1$ ($p2_1\,1\,1$, 9) 1; 2
[2] $p\,1\,1\,n$ ($p\,1\,1\,a$, 5) 1; 3

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pm2_1n$ ($\mathbf{a}'=3\mathbf{a}$) (32); [3] $pm2_1n$ ($\mathbf{b}'=3\mathbf{b}$) (32)

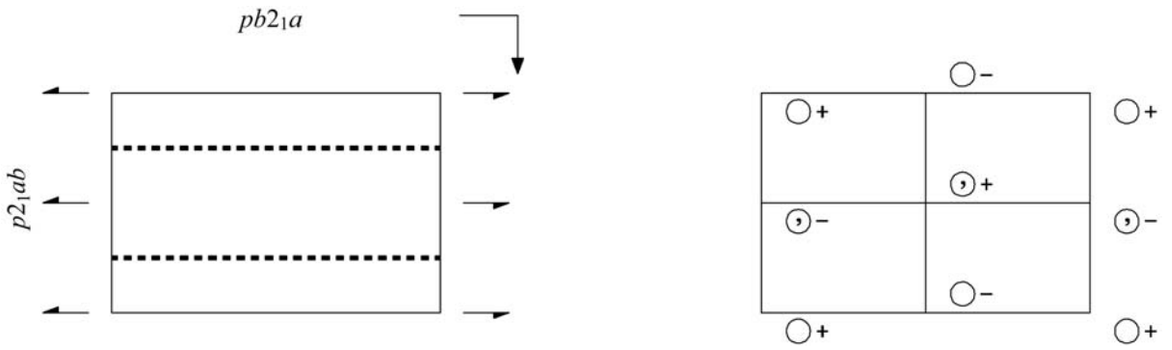
Minimal non-isotypic supergroups

I [2] $pman$ (42); [2] $pmmn$ (46)

II [2] $cm2m$ (35); [2] $pm2_1b$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (28); [2] $pm2a$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (31)

$pb2_1a$ $m2m$ Orthorhombic/Rectangular

No. 33 $pb2_1a$ Patterson symmetry $pmmm$



Origin on 12_1a

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (1|0,0,0)

(2) $2(0,\frac{1}{2},0)$ $0,y,0$ $(2_y|0,\frac{1}{2},0)$

(3) a $x,y,0$ $(m_z|\frac{1}{2},0,0)$

(4) b $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}$	(3) $x+\frac{1}{2},y,\bar{z}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hk : $h=2n$ $h0$: $h=2n$ $0k$: $k=2n$

Symmetry of special projections

Along [001] $p\,1\,g\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}\,2\,m\,g$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb\,1\,1$ (12) 1; 4
[2] $p\,1\,2_1\,1$ ($p2_1\,1\,1$, 9) 1; 2
[2] $p\,1\,1\,a$ (5) 1; 3

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pb2_1a$ ($\mathbf{a}'=3\mathbf{a}$) (33); [3] $pb2_1a$ ($\mathbf{b}'=3\mathbf{b}$) (33)

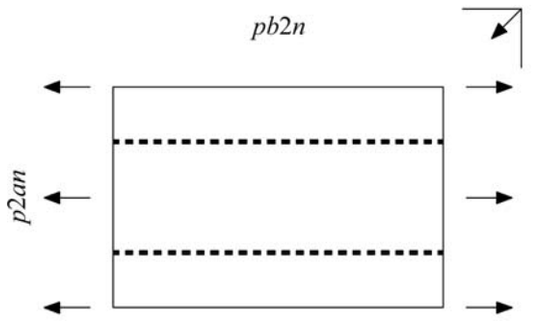
Minimal non-isotypic supergroups

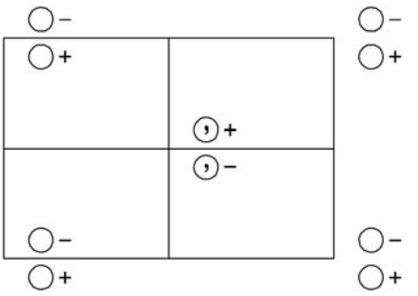
I [2] $pbaa$ (43); [2] $pbma$ (45)

II [2] $cm2e$ (36); [2] $p2_1am$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($pb2_1m$, 29); [2] $pm2a$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (31)

$pb2n$ $m2m$ Orthorhombic/Rectangular

No. 34 $pb2n$ Patterson symmetry $pmmm$





Origin on $12n$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1 (1\|0,0,0)
(2) 2 0,y,0 (2_y\|0,0,0)
(3) b $\frac{1}{4}$,y,z (m_x\|$\frac{1}{2}$,$\frac{1}{2}$,0)
(4) $n(\frac{1}{2},\frac{1}{2},0)$ x,y,0 (m_z\|$\frac{1}{2}$,$\frac{1}{2}$,0)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 b 1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	General: hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$ Special: no extra conditions
2 a .2.	$0,y,0$	$\frac{1}{2},y+\frac{1}{2},0$			

Symmetry of special projections

Along [001] $c1m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{m}2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb11$ (12) 1; 3
[2] $p121$ ($p211$, 8) 1; 2
[2] $p11n$ ($p11a$, 5) 1; 4

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pb2n$ ($\mathbf{a}'=3\mathbf{a}$) (34); [3] $pb2n$ ($\mathbf{b}'=3\mathbf{b}$) (34)

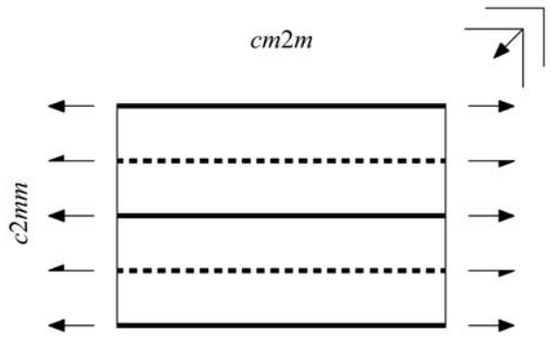
Minimal non-isotypic supergroups

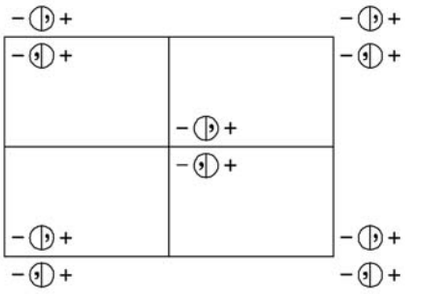
I [2] $pban$ (39); [2] $pman$ (42)

II [2] $cm2m$ (35); [2] $pb2b$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (30); [2] $pm2a$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (31)

$cm2m$ $m2m$ Orthorhombic/Rectangular

No. 35 $cm2m$ Patterson symmetry $cmmm$





Origin on $m2m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,y,0$ $(2_y|0,0,0)$

(3) $m \quad 0,y,z$ $(m_x|0,0,0)$

(4) $m \quad x,y,0$ $(m_z|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1|\frac{1}{2},\frac{1}{2},0)$

(2) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,0$ $(2_y|\frac{1}{2},\frac{1}{2},0)$

(3) $b \quad \frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

(4) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$ $(m_z|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	d	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},y,z$	(4) $x,y,\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: no extra conditions
4	c	$..m$	$x,y,0$	$\bar{x},y,0$			
4	b	$m..$	$0,y,z$	$0,y,\bar{z}$			
2	a	$m2m$	$0,y,0$				

Symmetry of special projections

Along [001] $c1m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] $cm11$ (13)	$(1;\ 3)+$
	[2] $c121$ ($c2\,1\,1$, 10)	$(1;\ 2)+$
	[2] $c11m$ ($p11m$, 4)	$(1;\ 4)+$
IIa	[2] $pb2n$ (34)	$1;\ 2;\ (3;\ 4)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $pm2_1n$ (32)	$1;\ 3;\ (2;\ 4)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $pb2_1m$ (29)	$1;\ 4;\ (2;\ 3)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $pm2m$ (27)	$1;\ 2;\ 3;\ 4$
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $cm2m$ ($\mathbf{a}'=3\mathbf{a}$) (35); [3] $cm2m$ ($\mathbf{b}'=3\mathbf{b}$) (35)

Minimal non-isotypic supergroups

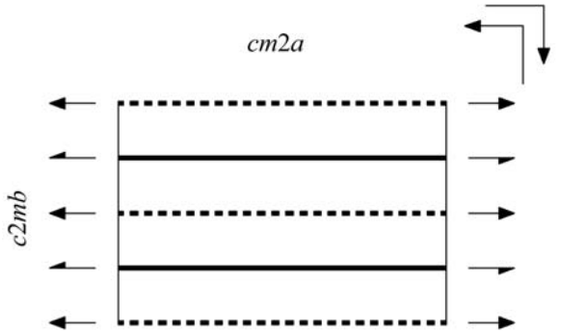
I [2] $cmmm$ (47)

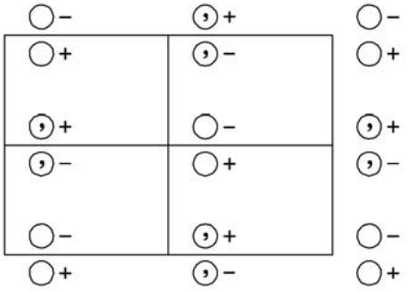
II [2] $pm2m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27)

*cm*2*e* *m*2*m* Orthorhombic/Rectangular

No. 36 *cm*2*e*

Patterson symmetry *cmmm*





Origin on *b*2*a*

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,y,0$	(3) m $\frac{1}{4},y,z$	(4) a $x,y,0$
$(1\|0,0,0)$	$(2_y\|0,0,0)$	$(m_x\|\frac{1}{2},0,0)$	$(m_z\|\frac{1}{2},0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(3) b $0,y,z$	(4) b $x,y,0$
$(1\|\frac{1}{2},\frac{1}{2},0)$	$(2_y\|\frac{1}{2},\frac{1}{2},0)$	$(m_x\|0,\frac{1}{2},0)$	$(m_z\|0,\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
8	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,z$	(4) $x+\frac{1}{2},y,\bar{z}$	General:
							hk: $h,k=2n$
							$h0$: $h=2n$
							$0k$: $k=2n$
							Special: no extra conditions
4	b	m . .	$\frac{1}{4},y,z$	$\frac{3}{4},y,\bar{z}$			
4	a	. 2 .	$0,y,0$	$\frac{1}{2},y,0$			

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{h}11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{h}2mg$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] $cm11$ (13)	(1; 3)+
	[2] $c121$ ($c211$, 10)	(1; 2)+
	[2] $c11a$ ($p11a$, 5)	(1; 4)+
IIa	[2] $pb2_1a$ (33)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pm2a$ (31)	1; 2; 3; 4
	[2] $pb2b$ (30)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pm2_1b$ (28)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $cm2e$ ($\mathbf{a}'=3\mathbf{a}$) (36); [3] $cm2e$ ($\mathbf{b}'=3\mathbf{b}$) (36)

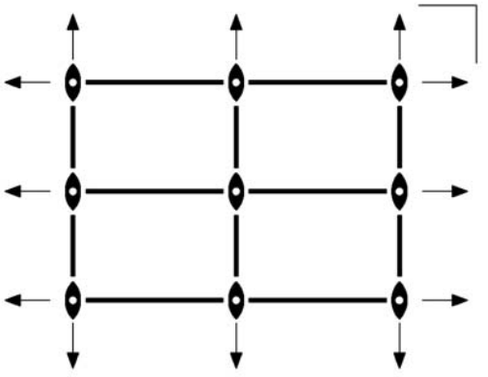
Minimal non-isotypic supergroups

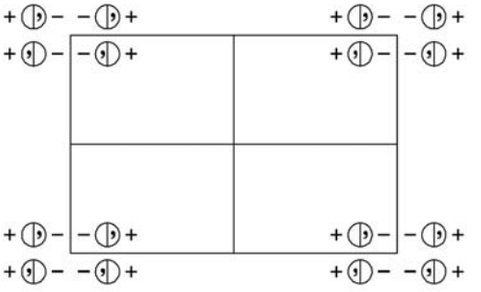
I [2] $cmme$ (48)

II [2] $pm2m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27)

$pmmm$ mmm Orthorhombic/Rectangular

No. 37 $p2/m2/m2/m$ Patterson symmetry $pmmm$





Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $2 \quad 0,y,0$
$(2_y|0,0,0)$

(4) $2 \quad x,0,0$
$(2_x|0,0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$
$(m_z|0,0,0)$

(7) $m \quad x,0,z$
$(m_y|0,0,0)$

(8) $m \quad 0,y,z$
$(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	r	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	no conditions
							Special: no extra conditions
4	q	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	
4	p	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x,\frac{1}{2},\bar{z}$	
4	o	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	
4	n	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	
4	m	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	
2	l	$mm2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	k	$mm2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	j	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	i	$mm2$	$0,0,z$	$0,0,\bar{z}$			
2	h	$m2m$	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	g	$m2m$	$0,y,0$	$0,\bar{y},0$			
2	f	$2mm$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	e	$2mm$	$x,0,0$	$\bar{x},0,0$			
1	d	mmm	$\frac{1}{2},\frac{1}{2},0$				
1	c	mmm	$0,\frac{1}{2},0$				
1	b	mmm	$\frac{1}{2},0,0$				
1	a	mmm	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $pm2m$ (27) 1; 3; 6; 8
[2] $p2mm$ ($pm2m$, 27) 1; 4; 6; 7
[2] $pmm2$ (23) 1; 2; 7; 8
[2] $p222$ (19) 1; 2; 3; 4
[2] $p12/m1$ ($p2/m11$, 14) 1; 3; 5; 7
[2] $p2/m11$ (14) 1; 4; 5; 8
[2] $p112/m$ (6) 1; 2; 5; 6

IIa none

IIb [2] $cmme$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (48); [2] $cmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (47); [2] $pmma$ ($\mathbf{a}' = 2\mathbf{a}$) (41); [2] $pmmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($pmma$, 41); [2] $pmam$ ($\mathbf{a}' = 2\mathbf{a}$) (40); [2] $pbmm$ ($\mathbf{b}' = 2\mathbf{b}$) ($pmam$, 40); [2] $pmaa$ ($\mathbf{a}' = 2\mathbf{a}$) (38); [2] $pbmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($pmaa$, 38)

Maximal isotypic subgroups of lowest index

IIc [2] $pmmm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (37)

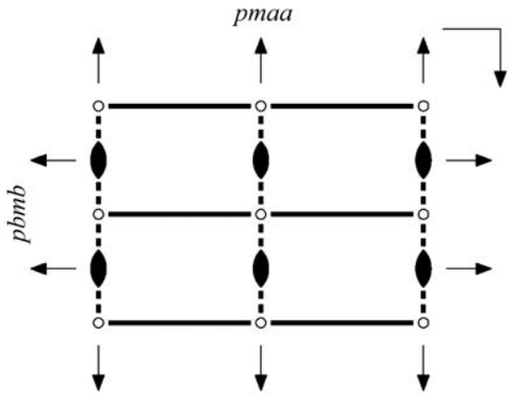
Minimal non-isotypic supergroups

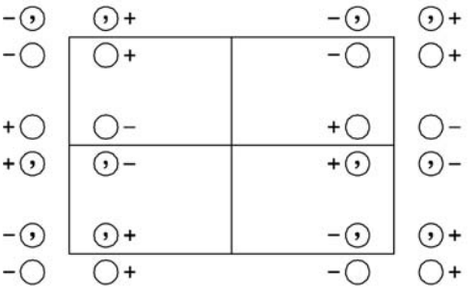
I [2] $p4/mmm$ (61)

II [2] $cmmm$ (47)

pmaa *mmm* Orthorhombic/Rectangular

No. 38 $p2/m2/a2/a$ Patterson symmetry $pmmm$





Origin at centre $(2/m)$ at $2/maa$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad x,0,0$
$(2_x|0,0,0)$

(3) $2 \quad \frac{1}{4},0,z$
$(2_z|\frac{1}{2},0,0)$

(4) $2 \quad \frac{1}{4},y,0$
$(2_y|\frac{1}{2},0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $m \quad 0,y,z$
$(m_x|0,0,0)$

(7) $a \quad x,y,0$
$(m_z|\frac{1}{2},0,0)$

(8) $a \quad x,0,z$
$(m_y|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	k	1	(1) x,y,z	(2) $x,\bar{y},\bar{z}$	(3) $\bar{x}+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,\bar{z}$	hk : $h=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $\bar{x},y,z$	(7) $x+\frac{1}{2},y,\bar{z}$	(8) $x+\frac{1}{2},\bar{y},z$	$h0$: $h=2n$
							Special: no extra conditions
4	j	m . .	$0,y,z$	$0,\bar{y},\bar{z}$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	
4	i	2 . .	$x,\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	
4	h	2 . .	$x,0,0$	$\bar{x}+\frac{1}{2},0,0$	$\bar{x},0,0$	$x+\frac{1}{2},0,0$	
4	g	. . 2	$\frac{1}{4},\frac{1}{2},z$	$\frac{1}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},\frac{1}{2},z$	
4	f	. . 2	$\frac{1}{4},0,z$	$\frac{1}{4},0,\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{3}{4},0,z$	
4	e	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},0$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,0$	
2	d	2 2 2	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$			
2	c	2 2 2	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$			
2	b	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	a	$2/m$ . .	$0,0,0$	$\frac{1}{2},0,0$			

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pm2a$ (31) 1; 4; 6; 7
[2] $p2aa$ ($pb2b$, 30) 1; 2; 7; 8
[2] $pma2$ (24) 1; 3; 6; 8
[2] $p222$ (19) 1; 2; 3; 4
[2] $p12/a1$ ($p2/b11$, 16) 1; 4; 5; 8
[2] $p2/m11$ (14) 1; 2; 5; 6
[2] $p112/a$ (7) 1; 3; 5; 7

IIa none

IIb [2] $pbaa$ ($\mathbf{b}' = 2\mathbf{b}$) (43); [2] $pman$ ($\mathbf{b}' = 2\mathbf{b}$) (42); [2] $pban$ ($\mathbf{b}' = 2\mathbf{b}$) (39)

Maximal isotypic subgroups of lowest index

IIc [2] $pmaa$ ($\mathbf{b}' = 2\mathbf{b}$) (38); [3] $pmaa$ ($\mathbf{a}' = 3\mathbf{a}$) (38)

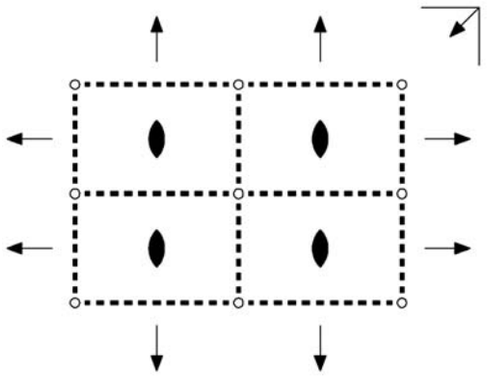
Minimal non-isotypic supergroups

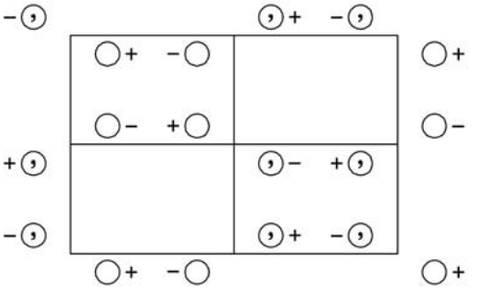
I none

II [2] $cmme$ (48); [2] $pmmm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (37)

pban *mmm* Orthorhombic/Rectangular

No. 39 $p2/b2/a2/n$ Patterson symmetry $pmmm$





Origin at $\bar{1}$ at *ban*, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from 222

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad \frac{1}{4}, \frac{1}{4}, z$
$(2_z|\frac{1}{2}, \frac{1}{2}, 0)$

(3) $2 \quad \frac{1}{4}, y, 0$
$(2_y|\frac{1}{2}, 0, 0)$

(4) $2 \quad x, \frac{1}{4}, 0$
$(2_x|0, \frac{1}{2}, 0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $n(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, 0$
$(m_z|\frac{1}{2}, \frac{1}{2}, 0)$

(7) $a \quad x, 0, z$
$(m_y|\frac{1}{2}, 0, 0)$

(8) $b \quad 0, y, z$
$(m_x|0, \frac{1}{2}, 0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y},z$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	g	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z$	no extra conditions
4	f	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	no extra conditions
4	e	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y+\frac{1}{2},0$	no extra conditions
4	d	2 . .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	no extra conditions
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	b	2 2 2	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			no extra conditions
2	a	2 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $\not{c}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb2n$ (34) 1; 3; 6; 8
[2] $p2an$ ($pb2n$, 34) 1; 4; 6; 7
[2] $pba2$ (25) 1; 2; 7; 8
[2] $p222$ (19) 1; 2; 3; 4
[2] $p12/a1$ ($p2/b11$, 16) 1; 3; 5; 7
[2] $p2/b11$ (16) 1; 4; 5; 8
[2] $p112/n$ ($p112/a$, 7) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pban$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (39)

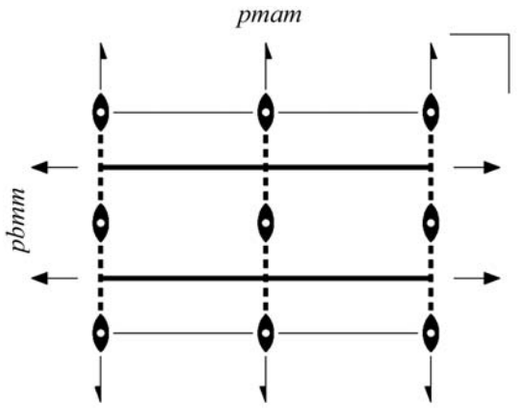
Minimal non-isotypic supergroups

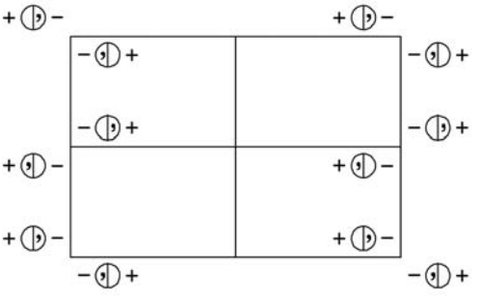
I [2] $p4/nbm$ (62)

II [2] $cmmm$ (47); [2] $pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (38)

$pmam$ mmm Orthorhombic/Rectangular

No. 40 $p2_1/m2/a2/m$ Patterson symmetry $pmmm$





Origin at centre $(2/m)$ at $2_1a2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad \frac{1}{4},y,0$
$(2_y|\frac{1}{2},0,0)$

(3) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(4) $2(\frac{1}{2},0,0) \quad x,0,0$
$(2_x|\frac{1}{2},0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $a \quad x,0,z$
$(m_y|\frac{1}{2},0,0)$

(7) $m \quad x,y,0$
$(m_z|0,0,0)$

(8) $m \quad \frac{1}{4},y,z$
$(m_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},\bar{y},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$	$h0$: $h=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},z$	(7) $x,y,\bar{z}$	(8) $\bar{x}+\frac{1}{2},y,z$	
							Special: as above, plus
4	g	m . .	$\frac{1}{4},y,z$	$\frac{1}{4},y,\bar{z}$	$\frac{3}{4},\bar{y},z$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	f	. . m	$x,y,0$	$\bar{x}+\frac{1}{2},y,0$	$\bar{x},\bar{y},0$	$x+\frac{1}{2},\bar{y},0$	no extra conditions
4	e	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hk: $h=2n$
4	d	. . 2	$0,0,z$	$\frac{1}{2},0,\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},0,z$	hk: $h=2n$
2	c	m 2 m	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$			no extra conditions
2	b	. . 2/m	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hk: $h=2n$
2	a	. . 2/m	$0,0,0$	$\frac{1}{2},0,0$			hk: $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $p2_1am$ ($pb2_1m$, 29) 1; 4; 6; 7
[2] $pm2m$ (27) 1; 2; 7; 8
[2] $pma2$ (24) 1; 3; 6; 8
[2] $p2_122$ (20) 1; 2; 3; 4
[2] $p12/a1$ ($p2/b11$, 16) 1; 2; 5; 6
[2] $p2_1/m11$ (15) 1; 4; 5; 8
[2] $p112/m$ (6) 1; 3; 5; 7

IIa none

IIb [2] $pmab$ ($\mathbf{b}'=2\mathbf{b}$) ($pbma$, 45); [2] $pbam$ ($\mathbf{b}'=2\mathbf{b}$) (44); [2] $pbab$ ($\mathbf{b}'=2\mathbf{b}$) ($pbaa$, 43)

Maximal isotypic subgroups of lowest index

IIc [2] $pmam$ ($\mathbf{b}'=2\mathbf{b}$) (40); [3] $pmam$ ($\mathbf{a}'=3\mathbf{a}$) (40)

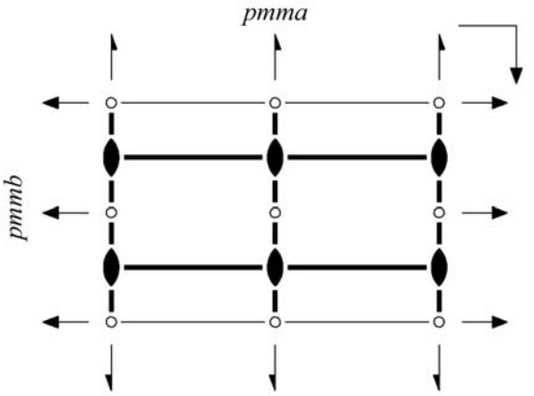
Minimal non-isotypic supergroups

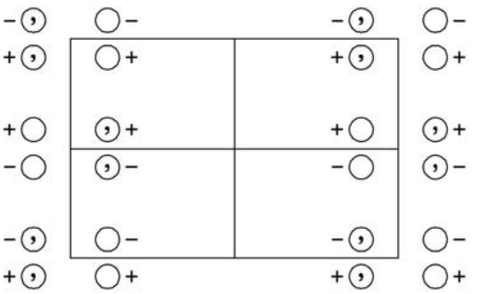
I none

II [2] $cmmm$ (47); [2] $pmmm$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (37)

$pmma$ mmm Orthorhombic/Rectangular

No. 41 $p2_1/m2/m2/a$ Patterson symmetry $pmmm$





Origin at centre $(2/m)$ at $2_12/ma$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad \frac{1}{4},0,z$
$(2_z|\frac{1}{2},0,0)$

(3) $2 \quad 0,y,0$
$(2_y|0,0,0)$

(4) $2(\frac{1}{2},0,0) \quad x,0,0$
$(2_x|\frac{1}{2},0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $a \quad x,y,0$
$(m_z|\frac{1}{2},0,0)$

(7) $m \quad x,0,z$
$(m_y|0,0,0)$

(8) $m \quad \frac{1}{4},y,z$
$(m_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*i*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$	hk : $h=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x}+\frac{1}{2},y,z$	$h0$: $h=2n$
							Special: no extra conditions
4	*h*	*m* . .	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y},z$	$\frac{3}{4},y,\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	
4	*g*	. *m* .	$x,\frac{1}{2},z$	$\bar{x}+\frac{1}{2},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\frac{1}{2},\bar{z}$	
4	*f*	. *m* .	$x,0,z$	$\bar{x}+\frac{1}{2},0,z$	$\bar{x},0,\bar{z}$	$x+\frac{1}{2},0,\bar{z}$	
4	*e*	. 2 .	$0,y,0$	$\frac{1}{2},\bar{y},0$	$0,\bar{y},0$	$\frac{1}{2},y,0$	
2	*d*	*m m* 2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			
2	*c*	*m m* 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			
2	*b*	. 2/*m* .	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	*a*	. 2/*m* .	$0,0,0$	$\frac{1}{2},0,0$			

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mg$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $pm2a$ (31) 1; 3; 6; 8
[2] $p2_1ma$ ($pm2_1b$, 28) 1; 4; 6; 7
[2] $pmm2$ (23) 1; 2; 7; 8
[2] $p2_122$ (20) 1; 2; 3; 4
[2] $p2_1/m11$ (15) 1; 4; 5; 8
[2] $p12/m1$ ($p2/m11$, 14) 1; 3; 5; 7
[2] $p112/a$ (7) 1; 2; 5; 6

IIa none

IIb [2] $pmmn$ ($\mathbf{b}' = 2\mathbf{b}$) (46); [2] $pbma$ ($\mathbf{b}' = 2\mathbf{b}$) (45); [2] $pbmn$ ($\mathbf{b}' = 2\mathbf{b}$) ($pman$, 42)

Maximal isotypic subgroups of lowest index

IIc [2] $pmma$ ($\mathbf{b}' = 2\mathbf{b}$) (41); [3] $pmma$ ($\mathbf{a}' = 3\mathbf{a}$) (41)

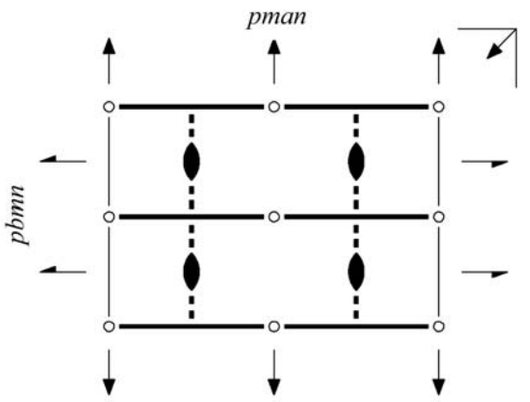
Minimal non-isotypic supergroups

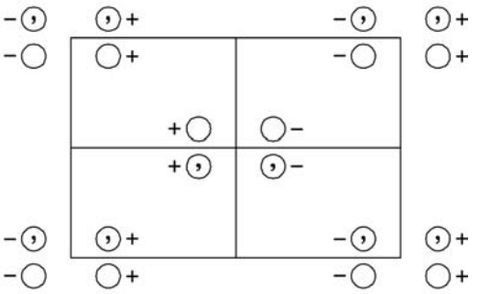
I none

II [2] $cmme$ (48); [2] $pmmm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (37)

$pman$ mmm Orthorhombic/Rectangular

No. 42 $p2/m2_1/a2/n$ Patterson symmetry $pmmm$





Origin at centre $(2/m)$ at $2/m1n$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(3) $2 \quad \frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(4) $2 \quad x,0,0$
$(2_x|0,0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $a \quad x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(7) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(8) $m \quad 0,y,z$
$(m_x|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (7) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hk : $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*e*	*m* . .	$0,y,z$	$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},z$	$0,\bar{y},\bar{z}$	no extra conditions
4	*d*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z$	hk : $h=2n$
4	*c*	2 . .	$x,0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},0,0$	$x+\frac{1}{2},\frac{1}{2},0$	no extra conditions
2	*b*	2/*m* . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions
2	*a*	2/*m* . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{c}2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $p2an$ ($pb2n$, 34) 1; 4; 6; 7
[2] $pm2_1n$ (32) 1; 2; 7; 8
[2] $pma2$ (24) 1; 3; 6; 8
[2] $p22_12$ ($p2_122$, 20) 1; 2; 3; 4
[2] $p12_1/a1$ ($p2_1/b11$, 17) 1; 2; 5; 6
[2] $p2/m11$ (14) 1; 4; 5; 8
[2] $p112/n$ ($p112/a$, 7) 1; 3; 5; 7

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pman$ ($\mathbf{a}' = 3\mathbf{a}$) (42); [3] $pman$ ($\mathbf{b}' = 3\mathbf{b}$) (42)

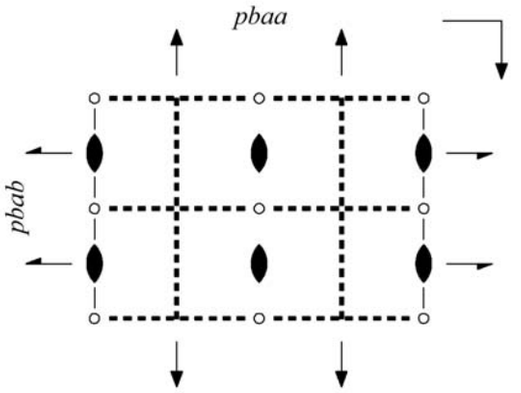
Minimal non-isotypic supergroups

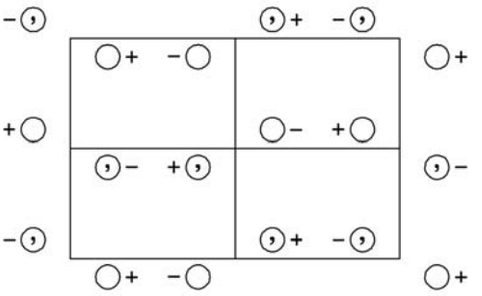
I none

II [2] $cmmm$ (47); [2] $pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (38); [2] $pmma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (41)

$pbaa$ mmm Orthorhombic/Rectangular

No. 43 $p2/b2_1/a2/a$ Patterson symmetry $pmmm$





Origin at $\bar{1}$ on $b1a$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad x,\frac{1}{4},0$ $(2_x|0,\frac{1}{2},0)$

(3) $2 \quad \frac{1}{4},0,z$ $(2_z|\frac{1}{2},0,0)$

(4) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,0$ $(2_y|\frac{1}{2},\frac{1}{2},0)$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $b \quad 0,y,z$ $(m_x|0,\frac{1}{2},0)$

(7) $a \quad x,y,0$ $(m_z|\frac{1}{2},0,0)$

(8) $a \quad x,\frac{1}{4},z$ $(m_y|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $x,\bar{y}+\frac{1}{2},\bar{z}$ (6) $\bar{x},y+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},\bar{y},z$ (7) $x+\frac{1}{2},y,\bar{z}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (8) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	hk: $h=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*c*	2 . .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{3}{4},0$	$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{1}{4},0$	no extra conditions
4	*b*	. . 2	$\frac{1}{4},0,z$	$\frac{1}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{3}{4},\frac{1}{2},z$	hk: $h+k=2n$
4	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},0$	hk: $h,k=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=-\frac{1}{2}\mathbf{a}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb2_1a$ (33) 1; 4; 6; 7
[2] $p2aa$ ($pb2b$, 30) 1; 2; 7; 8
[2] $pba2$ (25) 1; 3; 6; 8
[2] $p22_12$ ($p2_122$, 20) 1; 2; 3; 4
[2] $p12_1/a1$ ($p2_1/b11$, 17) 1; 4; 5; 8
[2] $p2/b11$ (16) 1; 2; 5; 6
[2] $p112/a$ (7) 1; 3; 5; 7

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pbaa$ ($\mathbf{a}'=3\mathbf{a}$) (43); [3] $pbaa$ ($\mathbf{b}'=3\mathbf{b}$) (43)

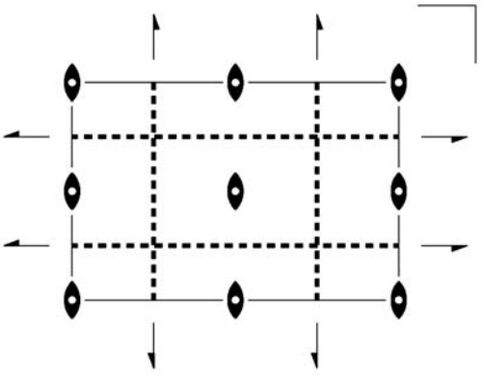
Minimal non-isotypic supergroups

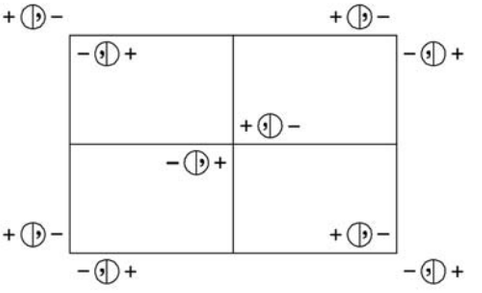
I none

II [2] $cmme$ (48); [2] $pmaa$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (38); [2] $pmam$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (40)

$pbam$ mmm Orthorhombic/Rectangular

No. 44 $p2_1/b2_1/a2/m$ Patterson symmetry $pmmm$





Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,0,z$ $(2_z|0,0,0)$

(3) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,0$ $(2_y|\frac{1}{2},\frac{1}{2},0)$

(4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$ $(m_z|0,0,0)$

(7) $a \quad x,\frac{1}{4},z$ $(m_y|\frac{1}{2},\frac{1}{2},0)$

(8) $b \quad \frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0k$: $k=2n$ $h0$: $h=2n$
							Special: as above, plus
4	*e*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
4	*d*	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hk : $h+k=2n$
4	*c*	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hk : $h+k=2n$
2	*b*	. . $2/m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk : $h+k=2n$
2	*a*	. . $2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk : $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I [2] $pb2_1m$ (29) 1; 3; 6; 8
[2] $p2_1am$ ($pb2_1m$, 29) 1; 4; 6; 7
[2] $pba2$ (25) 1; 2; 7; 8
[2] $p2_12_12$ (21) 1; 2; 3; 4
[2] $p12_1/a1$ ($p2_1/b11$, 17) 1; 3; 5; 7
[2] $p2_1/b11$ (17) 1; 4; 5; 8
[2] $p112/m$ (6) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pbam$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (44)

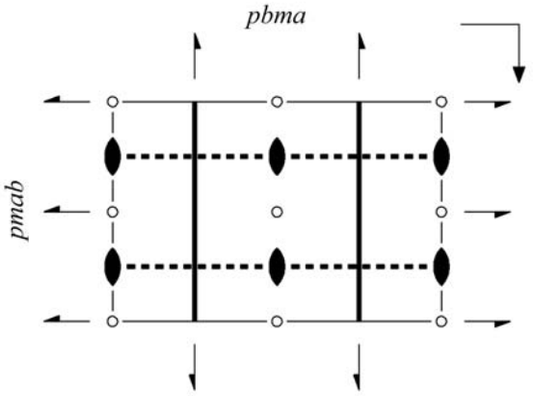
Minimal non-isotypic supergroups

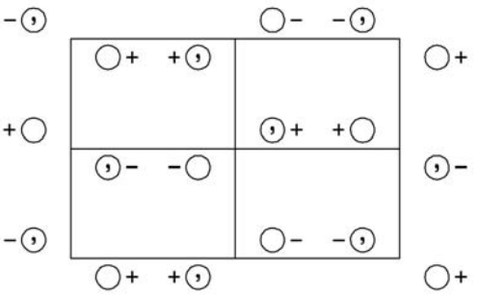
I [2] $p4/mbm$ (63)

II [2] $cmmm$ (47); [2] $pmam$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (40)

$pbma$ mmm Orthorhombic/Rectangular

No. 45 $p2_1/b2_1/m2/a$ Patterson symmetry $pmmm$





Origin at $\bar{1}$ on 12_1a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(0,\frac{1}{2},0)$ $0,y,0$ $(2_y|0,\frac{1}{2},0)$

(3) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

(4) 2 $\frac{1}{4},0,z$ $(2_z|\frac{1}{2},0,0)$

(5) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(6) m $x,\frac{1}{4},z$ $(m_y|0,\frac{1}{2},0)$

(7) b $\frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

(8) a $x,y,0$ $(m_z|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},y+\frac{1}{2},\bar{z}$ (6) $x,\bar{y}+\frac{1}{2},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (7) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},\bar{y},z$ (8) $x+\frac{1}{2},y,\bar{z}$	hk : $h=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*c*	. *m* .	$x,\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}$	$\bar{x}+\frac{1}{2},\frac{3}{4},z$	no extra conditions
4	*b*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$	hk : $k=2n$
4	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	hk : $k=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=-\frac{1}{2}\mathbf{a}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mg$
$\mathbf{a}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $pb2_1a$ (33) 1; 2; 7; 8
[2] $p2_1ma$ ($pm2_1b$, 28) 1; 3; 6; 8
[2] $pbm2$ ($pma2$, 24) 1; 4; 6; 7
[2] $p2_12_12$ (21) 1; 2; 3; 4
[2] $p2_1/b11$ (17) 1; 3; 5; 7
[2] $p12_1/m1$ ($p2_1/m11$, 15) 1; 2; 5; 6
[2] $p112/a$ (7) 1; 4; 5; 8

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pbma$ ($\mathbf{a}'=3\mathbf{a}$) (45); [3] $pbma$ ($\mathbf{b}'=3\mathbf{b}$) (45)

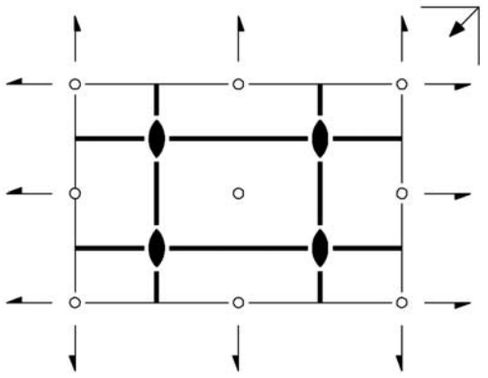
Minimal non-isotypic supergroups

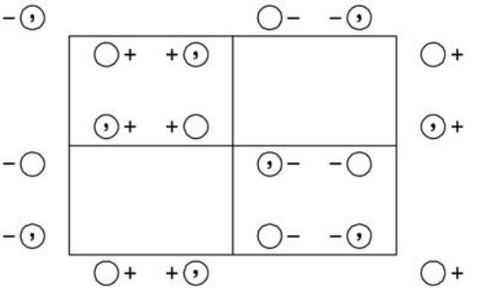
I none

II [2] $cmme$ (48); [2] $pmam$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (40); [2] $pmma$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (41)

$pmmn$ mmm Orthorhombic/Rectangular

No. 46 $p2_1/m2_1/m2/n$ Patterson symmetry $pmmm$





Origin at $\bar{1}$ on $2_1 2_1 n$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad \frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(3) $2(0,\frac{1}{2},0) \quad 0,y,0$
$(2_y|0,\frac{1}{2},0)$

(4) $2(\frac{1}{2},0,0) \quad x,0,0$
$(2_x|\frac{1}{2},0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(7) $m \quad x,\frac{1}{4},z$
$(m_y|0,\frac{1}{2},0)$

(8) $m \quad \frac{1}{4},y,z$
$(m_x|\frac{1}{2},0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*e*	. *m* .	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{3}{4},\bar{z}$	no extra conditions
4	*d*	*m* . .	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	*c*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hk: $h,k=2n$
2	*b*	*m m* 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			no extra conditions
2	*a*	*m m* 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $\not{c}2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}2mg$
$\mathbf{a}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I
[2] $pm2_1n$ (32) 1; 3; 6; 8
[2] $p2_1mn$ ($pm2_1n$, 32) 1; 4; 6; 7
[2] $pmm2$ (23) 1; 2; 7; 8
[2] $p2_12_12$ (21) 1; 2; 3; 4
[2] $p12_1/m1$ ($p2_1/m11$, 15) 1; 3; 5; 7
[2] $p2_1/m11$ (15) 1; 4; 5; 8
[2] $p112/n$ ($p112/a$, 7) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $pmmn$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (46)

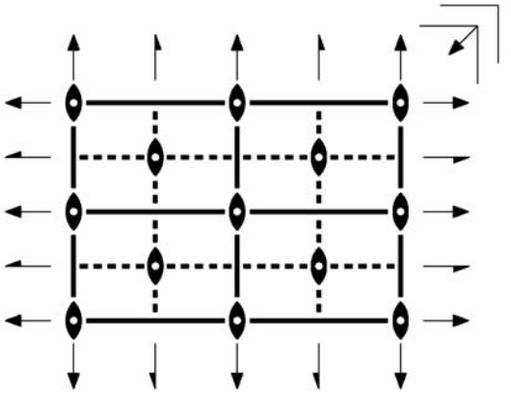
Minimal non-isotypic supergroups

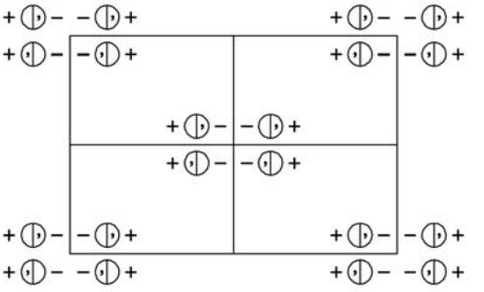
I [2] $p4/nmm$ (64)

II [2] $cmmm$ (47); [2] $pmma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (41)

cmmm *mmm* Orthorhombic/Rectangular

No. 47 *c*2/*m*2/*m*2/*m* Patterson symmetry *cmmm*





Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 2 $0,y,0$
$(2_y|0,0,0)$

(4) 2 $x,0,0$
$(2_x|0,0,0)$

(5) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(6) m $x,y,0$
$(m_z|0,0,0)$

(7) m $x,0,z$
$(m_y|0,0,0)$

(8) m $0,y,z$
$(m_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$
$(1|\frac{1}{2},\frac{1}{2},0)$

(2) 2 $\frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
$(2_x|\frac{1}{2},\frac{1}{2},0)$

(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
$(\bar{1}|\frac{1}{2},\frac{1}{2},0)$

(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(7) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(8) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
16	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
8	k	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	j	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	i	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	h	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	hk: $h=2n$
4	g	$m\,m\,2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	f	$m\,m\,2$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	e	$m\,2\,m$	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	d	$2\,m\,m$	$x,0,0$	$\bar{x},0,0$			no extra conditions
4	c	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hk: $h=2n$
2	b	$m\,m\,m$	$\frac{1}{2},0,0$				no extra conditions
2	a	$m\,m\,m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{c}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not{c}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] $cm2m$ (35)	(1; 3; 6; 8)+
	[2] $c2mm$ ($cm2m$, 35)	(1; 4; 6; 7)+
	[2] $cmm2$ (26)	(1; 2; 7; 8)+
	[2] $c222$ (22)	(1; 2; 3; 4)+
	[2] $c12/m1$ ($c2/m11$, 18)	(1; 3; 5; 7)+
	[2] $c2/m11$ (18)	(1; 4; 5; 8)+
	[2] $c112/m$ ($p112/m$, 6)	(1; 2; 5; 6)+
IIa	[2] $pmmn$ (46)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pbam$ (44)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pbmn$ ($pman$, 42)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pman$ (42)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pmam$ (40)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pbmm$ ($pmam$, 40)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pban$ (39)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $pmmm$ (37)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $cmmm$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (47)

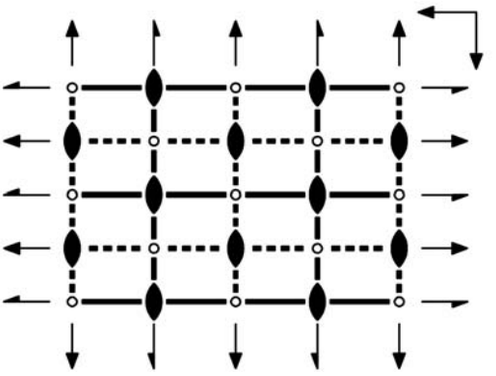
Minimal non-isotypic supergroups

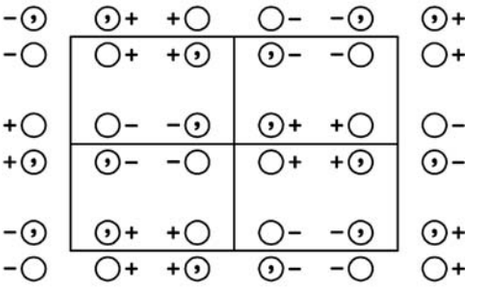
I [2] $p4/mmm$ (61); [2] $p4/mbm$ (63); [3] $p6/mmm$ (80)

II [2] $pmmm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (37)

cmme *mmm* Orthorhombic/Rectangular

No. 48 $c2/m2/m2/e$ Patterson symmetry $cmmm$





Origin at centre $(2/m)$ at $2/m2_1/ae$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $(1|0,0,0)$

(2) $2 \quad 0,\frac{1}{4},z$ $(2_z|0,\frac{1}{2},0)$

(3) $2(0,\frac{1}{2},0) \quad 0,y,0$ $(2_y|0,\frac{1}{2},0)$

(4) $2 \quad x,0,0$ $(2_x|0,0,0)$

(5) $\bar{1} \quad 0,0,0$ $(\bar{1}|0,0,0)$

(6) $b \quad x,y,0$ $(m_z|0,\frac{1}{2},0)$

(7) $m \quad x,\frac{1}{4},z$ $(m_y|0,\frac{1}{2},0)$

(8) $m \quad 0,y,z$ $(m_x|0,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $(1|\frac{1}{2},\frac{1}{2},0)$

(2) $2 \quad \frac{1}{4},0,z$ $(2_z|\frac{1}{2},0,0)$

(3) $2 \quad \frac{1}{4},y,0$ $(2_y|\frac{1}{2},0,0)$

(4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$ $(2_x|\frac{1}{2},\frac{1}{2},0)$

(5) $\bar{1} \quad \frac{1}{4},\frac{1}{4},0$ $(\bar{1}|\frac{1}{2},\frac{1}{2},0)$

(6) $a \quad x,y,0$ $(m_z|\frac{1}{2},0,0)$

(7) $a \quad x,0,z$ $(m_y|\frac{1}{2},0,0)$

(8) $b \quad \frac{1}{4},y,z$ $(m_x|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			
16	*j*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$
8	*i*	. *m* .	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$
8	*h*	*m* . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$
8	*g*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$
8	*f*	. 2 .	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{1}{4},y+\frac{1}{2},0$
8	*e*	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$
4	*d*	*m m* 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$		
4	*c*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$		
4	*b*	2/*m* . .	$0,0,0$	$0,\frac{1}{2},0$		
4	*a*	2 2 2	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$		

Reflection conditions

General:

hk: $h,k=2n$
$h0$: $h=2n$
$0k$: $k=2n$

Special: no extra conditions

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [010] $\not p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isotypic subgroups

I	[2] *cm*2*e* (36)	(1; 3; 6; 8)+
	[2] *c*2*me* (*cm*2*e*, 36)	(1; 4; 6; 7)+
	[2] *cmm*2 (26)	(1; 2; 7; 8)+
	[2] *c*222 (22)	(1; 2; 3; 4)+
	[2] *c*12/*m*1 (*c*2/*m*11, 18)	(1; 3; 5; 7)+
	[2] *c*2/*m*11 (18)	(1; 4; 5; 8)+
	[2] *c*112/*b* (*p*112/*a*, 7)	(1; 2; 5; 6)+
IIa	[2] *pbma* (45)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pmab* (*pbma*, 45)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pbaa* (43)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pbab* (*pbaa*, 43)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pmmb* (*pmma*, 41)	1; 2; 3; 4; 5; 6; 7; 8
	[2] *pmma* (41)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pmaa* (38)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *pbmb* (*pmaa*, 38)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] *cmme* ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (48)

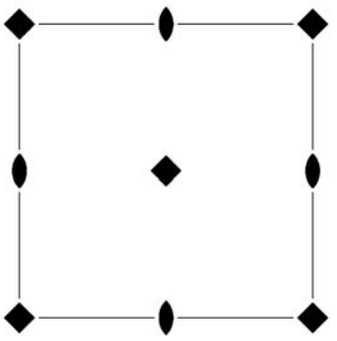
Minimal non-isotypic supergroups

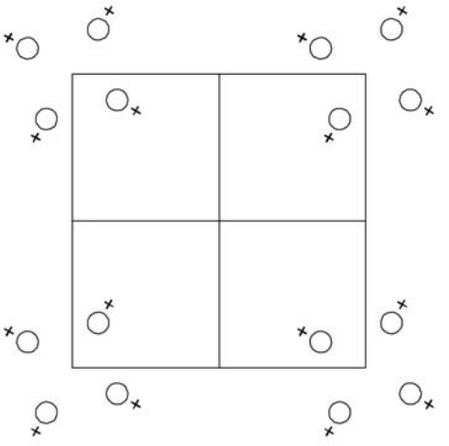
I [2] $p4/nbm$ (62); [2] $p4/nmm$ (64)

II [2] *pmmm* ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (37)

$p4$ 4 Tetragonal/Square

No. 49 $p4$ Patterson symmetry $p4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	c	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			$hk:\ h+k=2n$
1	b	4 . .	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 . .	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p211$ ($p112$, 3) 1; 2
IIa none
IIb none

Maximal isotypic subgroups of lowest index

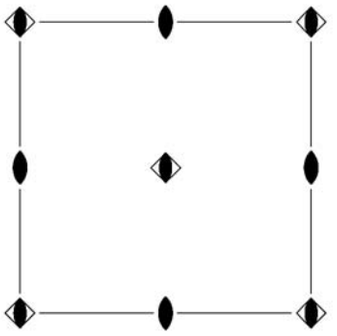
IIc [2] $c4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4$, 49)

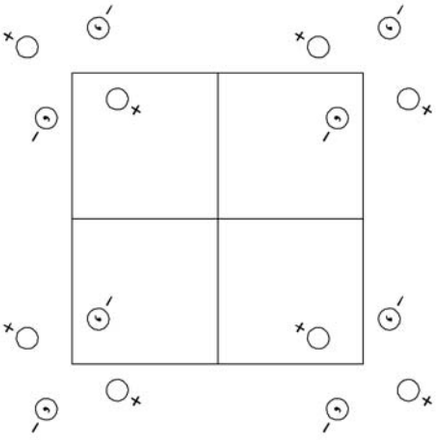
Minimal non-isotypic supergroups

I [2] $p4/m$ (51); [2] $p4/n$ (52); [2] $p422$ (53); [2] $p4_{1}22$ (54); [2] $p4mm$ (55); [2] $p4bm$ (56)
II none

$p\bar{4}$ $\bar{4}$ Tetragonal/Square

No. 50 $p\bar{4}$ Patterson symmetry $p4/m$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z$; $0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	no conditions
							Special:
2	e	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk:\ h+k=2n$
2	d	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	c	2 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	b	$\bar{4}$ . .	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$\bar{4}$ . .	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}1m1$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{m}1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p211$ ($p112$, 3) 1; 2
IIa none
IIb none

Maximal isotypic subgroups of lowest index

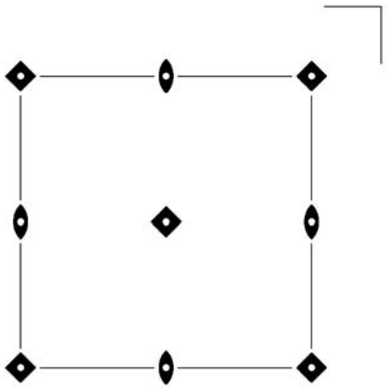
IIc [2] $c\bar{4}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($p\bar{4}$, 50)

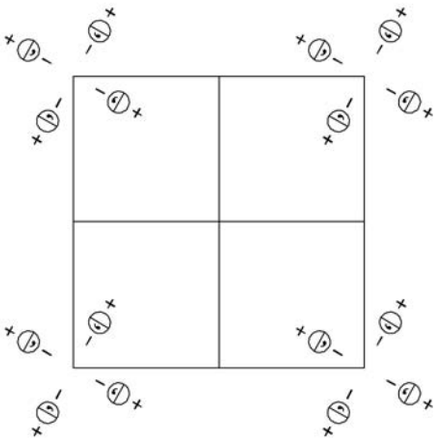
Minimal non-isotypic supergroups

I [2] $p4/m$ (51); [2] $p4/n$ (52); [2] $p\bar{4}2m$ (57); [2] $p\bar{4}2_1m$ (58); [2] $p\bar{4}m2$ (59); [2] $p\bar{4}b2$ (60)
II none

$p4/m$ $4/m$ Tetragonal/Square

No. 51 $p4/m$ Patterson symmetry $p4/m$





Origin at centre $(4/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \quad 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \quad 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(6) $m \quad x,y,0$
$(m_z|0,0,0)$

(7) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z|0,0,0)$

(8) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	no conditions
							Special:
4	g	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$hk:\ h+k=2n$
2	e	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	d	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	c	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			$hk:\ h+k=2n$
1	b	$4/m$ . .	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$4/m$ . .	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}$ (50) 1; 2; 7; 8
[2] $p4$ (49) 1; 2; 3; 4
[2] $p2/m11$ ($p112/m$, 6) 1; 2; 5; 6

IIa none

IIb [2] $c4/a$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($p4/n$, 52)

Maximal isotypic subgroups of lowest index

IIc [2] $c4/m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($p4/m$, 51)

Minimal non-isotypic supergroups

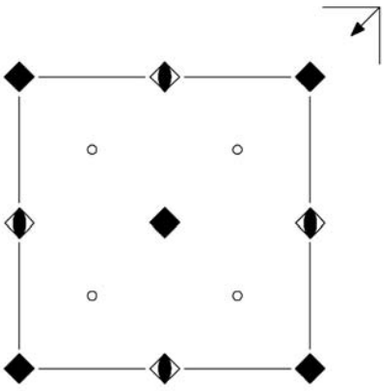
I [2] $p4/mmm$ (61); [2] $p4/mbm$ (63)

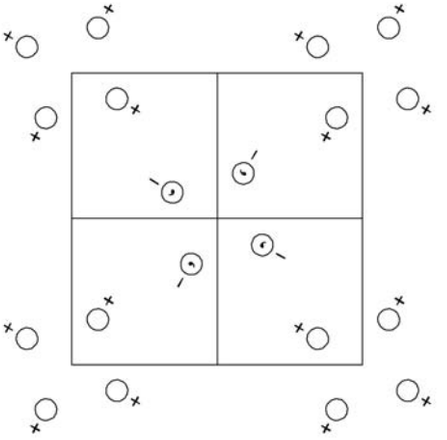
II none

$p4/n$ $4/m$ Tetragonal/Square

No. 52 $p4/n$ Patterson symmetry $p4/m$

ORIGIN CHOICE 1





Origin at 4 on n at $-\frac{1}{4},-\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \; 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \; 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $\bar{1} \quad \frac{1}{4},\frac{1}{4},0$
$(\bar{1}|\frac{1}{2},\frac{1}{2},0)$

(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(7) $\bar{4}^+ \; \frac{1}{2},0,z; \; \frac{1}{2},0,0$
$(\bar{4}_z|\frac{1}{2},\frac{1}{2},0)$

(8) $\bar{4}^- \; \frac{1}{2},0,z; \; \frac{1}{2},0,0$
$(\bar{4}_z^{-1}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	d	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hk: $h,k=2n$
2	b	4 . .	$\frac{1}{2},\frac{1}{2},z$	$0,0,\bar{z}$			no extra conditions
2	a	$\bar{4}$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}$ (50) 1; 2; 7; 8
[2] $p4$ (49) 1; 2; 3; 4
[2] $p2/n11$ ($p112/a$, 7) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

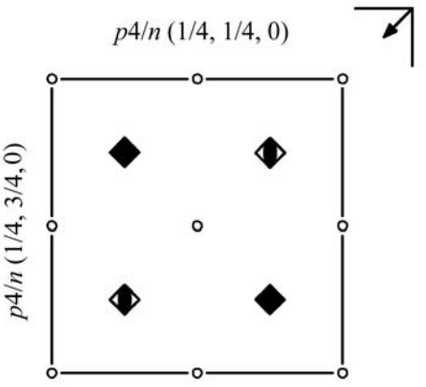
IIc [5] $p4/n$ ($\mathbf{a}' = \mathbf{a}+2\mathbf{b}, \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}-2\mathbf{b}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$) (52)

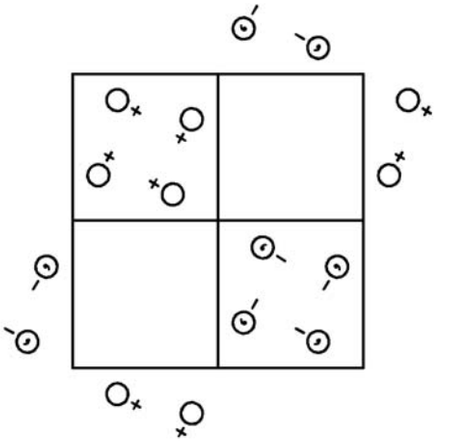
Minimal non-isotypic supergroups

I [2] $p4/nbm$ (62); [2] $p4/nmm$ (64)

II [2] $c4/m$ ($p4/m$, 51)

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n at $\frac{1}{4},\frac{1}{4},0$ from 4

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $\frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(3) 4^+ $\frac{1}{4},\frac{1}{4},z$
$(4_z|\frac{1}{2},0,0)$

(4) 4^- $\frac{1}{4},\frac{1}{4},z$
$(4_z^{-1}|0,\frac{1}{2},0)$

(5) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(7) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;$ $\frac{1}{4},-\frac{1}{4},0$
$(\bar{4}_z|\frac{1}{2},0,0)$

(8) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;$ $-\frac{1}{4},\frac{1}{4},0$
$(\bar{4}_z^{-1}|0,\frac{1}{2},0)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x,z$ (7) $y+\frac{1}{2},\bar{x},\bar{z}$	(4) $y,\bar{x}+\frac{1}{2},z$ (8) $\bar{y},x+\frac{1}{2},\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	d	2 . .	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	no extra conditions
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	b	4 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	a	$\bar{4}$ . .	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}$ (50) 1; 2; 7; 8
[2] $p4$ (49) 1; 2; 3; 4
[2] $p2/n11$ ($p112/a$, 7) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [5] $p4/n$ ($\mathbf{a}' = \mathbf{a}+2\mathbf{b}, \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}-2\mathbf{b}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$) (52)

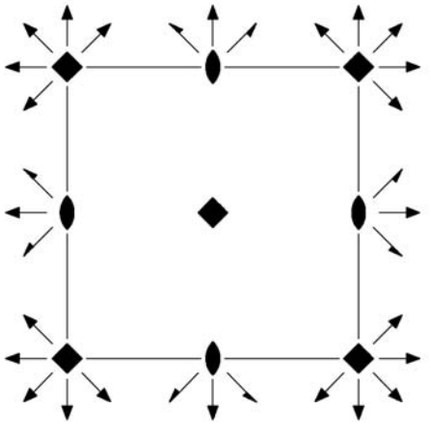
Minimal non-isotypic supergroups

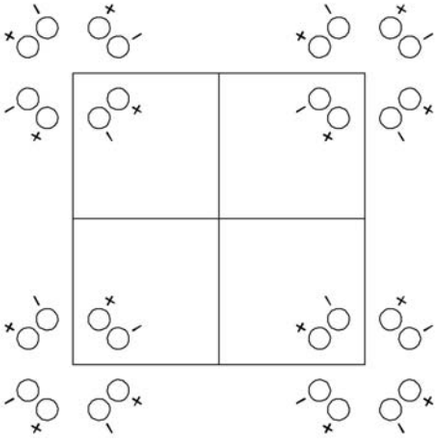
I [2] $p4/nbm$ (62); [2] $p4/nmm$ (64)

II [2] $c4/m$ ($p4/m$, 51)

$p422$ 422 Tetragonal/Square

No. 53 $p422$ Patterson symmetry $p4/mmm$





Origin at 422

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	j	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	i	. 2 .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	h	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	g	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hk : $h+k=2n$
2	e	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	d	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	c	2 22 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hk : $h,k=2n$
1	b	4 2 2	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	4 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p411$ ($p4$, 49) 1; 2; 3; 4
[2] $p212$ ($c222$, 22) 1; 2; 7; 8
[2] $p221$ ($p222$, 19) 1; 2; 5; 6

IIa none

IIb [2] $c422_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p42_12$, 54)

Maximal isotypic subgroups of lowest index

IIc [2] $c422$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p422$, 53)

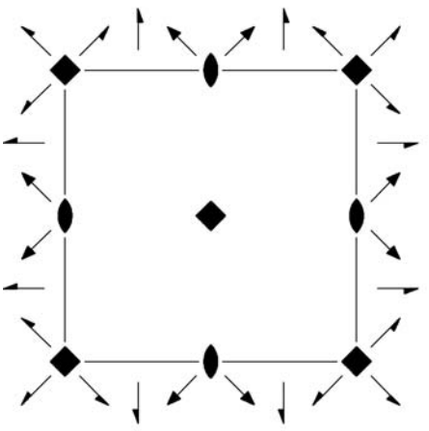
Minimal non-isotypic supergroups

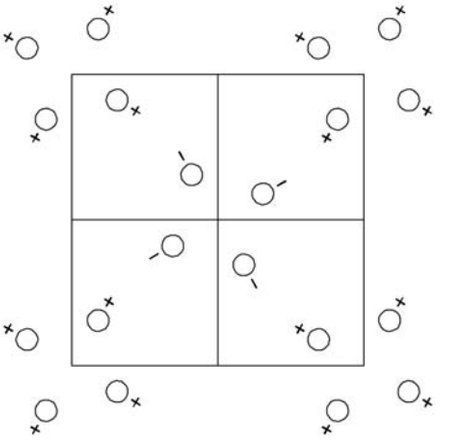
I [2] $p4/mmm$ (61); [2] $p4/nbm$ (62)

II none

$p42_12$ 422 Tetragonal/Square

No. 54 $p42_12$ Patterson symmetry $p4/mmm$





Origin on 4 at $-\frac{1}{2},0,0$ from 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
$(2_x|\frac{1}{2},\frac{1}{2},0)$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
$(2_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) $2(\frac{1}{2},\frac{1}{2},0)$ $x,\bar{x},0$
$(2_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	d	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	c	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hk: $h+k=2n$
2	b	4 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			hk: $h+k=2n$
2	a	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk: $h+k=2n$

Symmetry of special projections

Along [001] $p\,4\,g\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p\,2\,m\,g$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $\not p\,2\,m\,m$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\,4\,1\,1$ ($p4$, 49) 1; 2; 3; 4
[2] $p\,2\,1\,2$ ($c\,2\,2\,2$, 22) 1; 2; 7; 8
[2] $p\,2\,2_1\,1$ ($p\,2_1\,2_1\,2$, 21) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p\,4\,2_1\,2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (54)

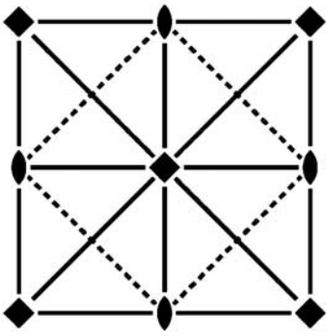
Minimal non-isotypic supergroups

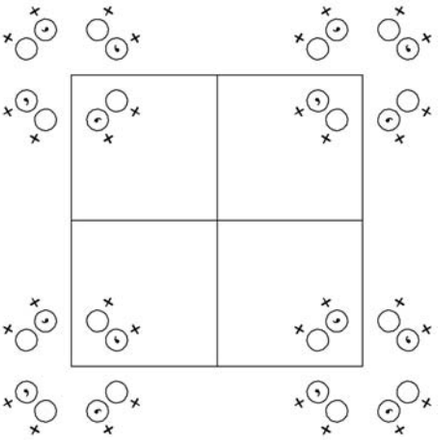
I [2] $p\,4/m\,b\,m$ (63); [2] $p\,4/n\,m\,m$ (64)

II [2] $c\,4\,2\,2$ ($p\,4\,2\,2$, 53)

$p4mm$ $4mm$ Tetragonal/Square

No. 55 $p4mm$ Patterson symmetry $p4/mmm$





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \quad 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \quad 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $m \quad x,0,z$
$(m_y|0,0,0)$

(6) $m \quad 0,y,z$
$(m_x|0,0,0)$

(7) $m \quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) $m \quad x,x,z$
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	no conditions
							Special:
4	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	. m .	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	. . m	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	2 mm .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hk : $h+k=2n$
1	b	4 m m	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 m m	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not/\!/ 1m1$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $\not/\!/ 1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p4\,1\,1$ ($p4$, 49) 1; 2; 3; 4
[2] $p2\,1\,m$ ($cmm2$, 26) 1; 2; 7; 8
[2] $p2m\,1$ ($pmm2$, 23) 1; 2; 5; 6

IIa none

IIb [2] $c4md$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4bm$, 56)

Maximal isotypic subgroups of lowest index

IIc [2] $c4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4mm$, 55)

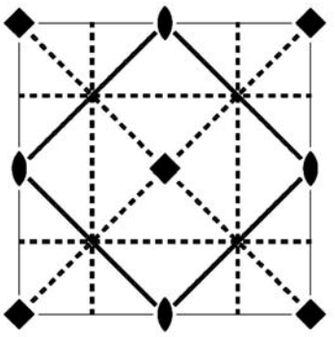
Minimal non-isotypic supergroups

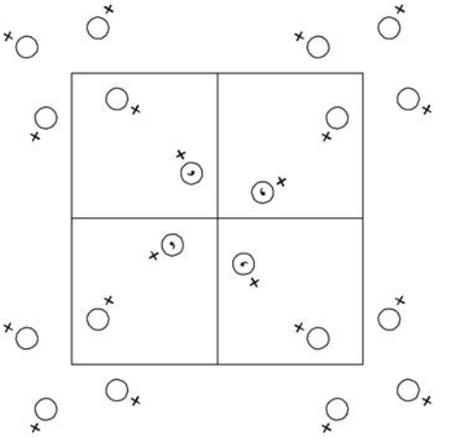
I [2] $p4/mmm$ (61); [2] $p4/nmm$ (64)

II none

$p4bm$ $4mm$ Tetragonal/Square

No. 56 $p4bm$ Patterson symmetry $p4/mmm$





Origin on $41g$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad y \le \frac{1}{2} - x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(6) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

(7) m $x+\frac{1}{2},\bar{x},z$
$(m_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
$(m_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x},z$ (8) $y+\frac{1}{2},x+\frac{1}{2},z$	$0k$: $k=2n$ $h0$: $h=2n$
							Special: as above, plus
4	c	. . m	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
2	b	2 . mm	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hk : $h+k=2n$
2	a	4 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hk : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p411$ ($p4$, 49) 1; 2; 3; 4
[2] $p21m$ ($cmm2$, 26) 1; 2; 7; 8
[2] $p2b1$ ($pba2$, 25) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4bm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (56)

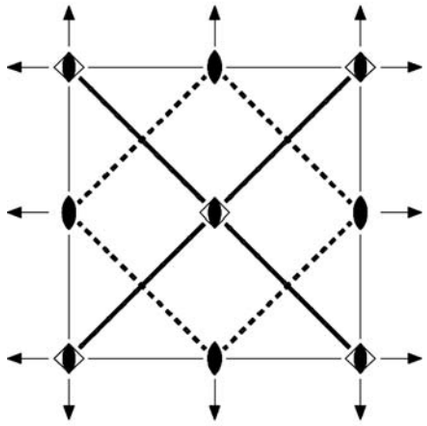
Minimal non-isotypic supergroups

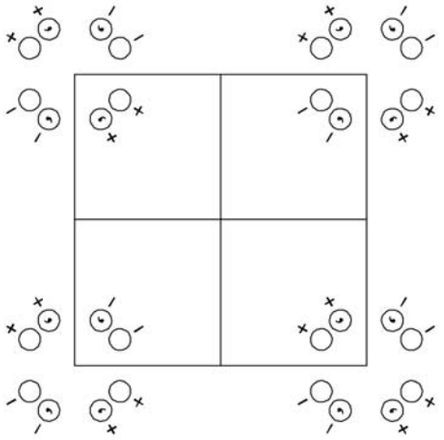
I [2] $p4/nbm$ (62); [2] $p4/mbm$ (63)

II [2] $c4mm$ ($p4mm$, 55)

$p\bar{4}2m$ $\bar{4}2m$ Tetragonal/Square

No. 57 $p\bar{4}2m$ Patterson symmetry $p4/mmm$





Origin at $\bar{4}2m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;$ $0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;$ $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m x,x,z
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	j	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	no conditions
							Special:
4	i	. . m	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
4	h	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	$hk:\ h+k=2n$
4	g	. 2 .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},\bar{x},0$	$\frac{1}{2},x,0$	no extra conditions
4	f	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
2	e	2 . mm	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	d	2 . mm	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	c	2 22 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			$hk:\ h+k=2n$
1	b	$\bar{4}$ 2 m	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$\bar{4}$ 2 m	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not/2mm$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not/1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 50) 1; 2; 3; 4
[2] $p21m$ ($cmm2$, 26) 1; 2; 7; 8
[2] $p221$ ($p222$, 19) 1; 2; 5; 6

IIa none

IIb [2] $c\bar{4}2d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($p\bar{4}b2$, 60); [2] $c\bar{4}2m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($p\bar{4}m2$, 59)

Maximal isotypic subgroups of lowest index

IIc [9] $p\bar{4}2m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (57)

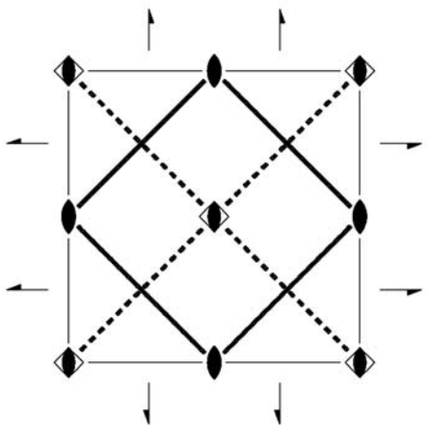
Minimal non-isotypic supergroups

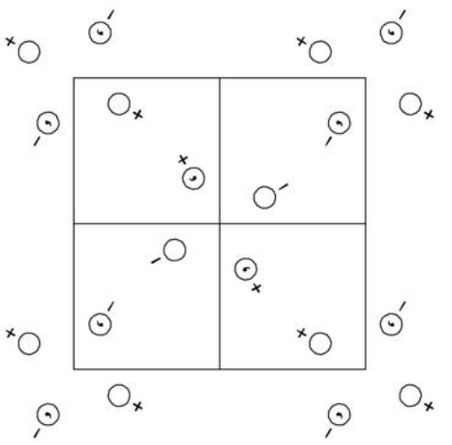
I [2] $p4/mmm$ (61); [2] $p4/nbm$ (62)

II [2] $c\bar{4}2m$ ($p\bar{4}m2$, 59)

$p\bar{4}2_1m$ $\bar{4}2m$ Tetragonal/Square

No. 58 $p\bar{4}2_1m$ Patterson symmetry $p4/mmm$





Origin at $\bar{4}1g$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad y \le \frac{1}{2} - x$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z$; $0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
$(2_x|\frac{1}{2},\frac{1}{2},0)$

(7) m $x+\frac{1}{2},\bar{x},z$
$(m_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
$(m_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $\bar{y},x,\bar{z}$ (8) $y+\frac{1}{2},x+\frac{1}{2},z$	$h0$: $h=2n$
							Special: as above, plus
4	d	. . m	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,\bar{z}$	no extra conditions
4	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hk: $h+k=2n$
2	b	2 . mm	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			hk: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk: $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $\not{p}1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 50) 1; 2; 3; 4
[2] $p21m$ ($cmm2$, 26) 1; 2; 7; 8
[2] $p22_11$ ($p2_12_12$, 21) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p\bar{4}2_1m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (58)

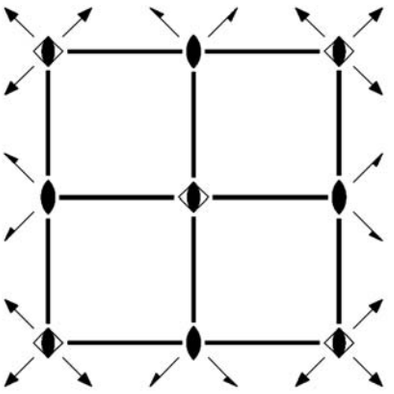
Minimal non-isotypic supergroups

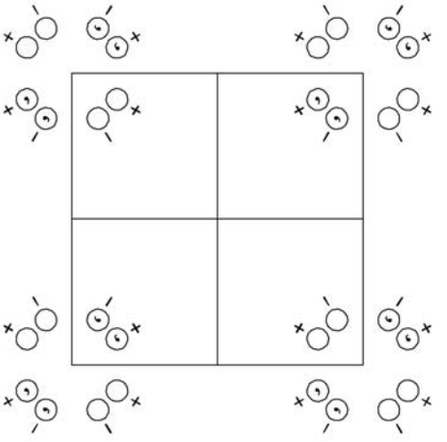
I [2] $p4/mbm$ (63); [2] $p4/nmm$ (64)

II [2] $c\bar{4}2m$ ($p\bar{4}m2$, 59)

$p\bar{4}m2$ $\bar{4}m2$ Tetragonal/Square

No. 59 $p\bar{4}m2$ Patterson symmetry $p4/mmm$





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z;\ 0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z;\ 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) m $x,0,z$
$(m_y|0,0,0)$

(6) m $0,y,z$
$(m_x|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	h	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},\bar{x},\bar{z}$	$\frac{1}{2},x,\bar{z}$	no extra conditions
4	g	. m .	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$	no extra conditions
4	f	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$	no extra conditions
2	e	2 mm .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			hk : $h+k=2n$
2	d	2 mm .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	c	2 mm .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	b	$\bar{4}$ m 2	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$\bar{4}$ m 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 50) 1; 2; 3; 4
[2] $p2m1$ ($pmm2$, 23) 1; 2; 5; 6
[2] $p212$ ($c222$, 22) 1; 2; 7; 8

IIa none

IIb [2] $c\bar{4}m2_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p\bar{4}2_1m$, 58); [2] $c\bar{4}m2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p\bar{4}2m$, 57)

Maximal isotypic subgroups of lowest index

IIc [9] $p\bar{4}m2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (59)

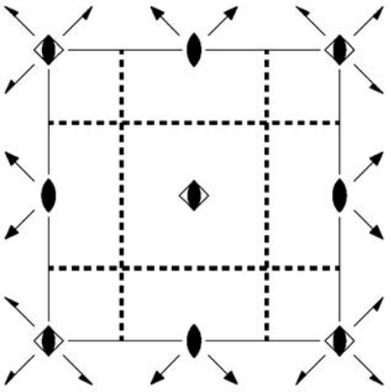
Minimal non-isotypic supergroups

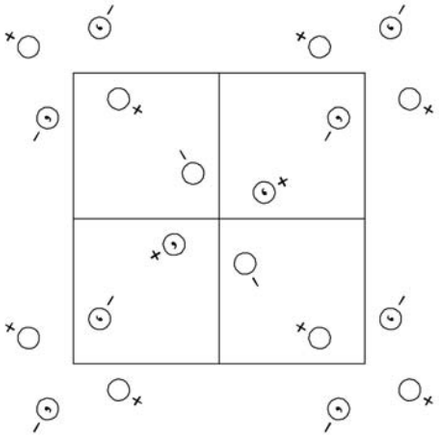
I [2] $p4/mmm$ (61); [2] $p4/nmm$ (64)

II [2] $c\bar{4}m2$ ($p\bar{4}2m$, 57)

$p\bar{4}b2$ $\bar{4}m2$ Tetragonal/Square

No. 60 $p\bar{4}b2$ Patterson symmetry $p4/mmm$





Origin at $\bar{4}12_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) $\bar{4}^+$ $0,0,z$; $0,0,0$
$(\bar{4}_z|0,0,0)$

(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(5) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(6) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
$(2_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) 2 $x,\bar{x}+\frac{1}{2},0$
$(2_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	$h0$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
							Special: as above, plus
4	e	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
4	d	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	hk: $h+k=2n$
4	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hk: $h+k=2n$
2	b	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk: $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 50) 1; 2; 3; 4
[2] $p2b1$ ($pba2$, 25) 1; 2; 5; 6
[2] $p212$ ($c222$, 22) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p\bar{4}b2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (60)

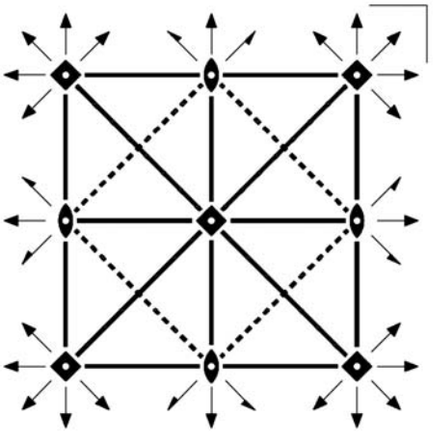
Minimal non-isotypic supergroups

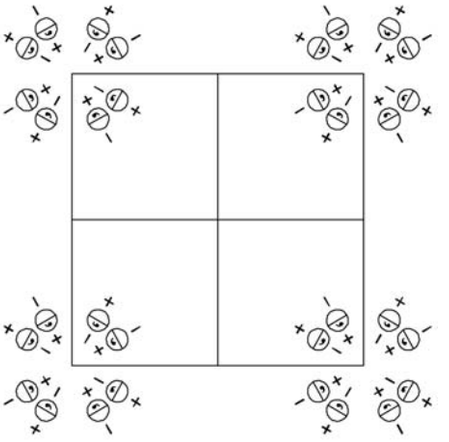
I [2] $p4/nbm$ (62); [2] $p4/mbm$ (63)

II [2] $c\bar{4}m2$ ($p\bar{4}2m$, 57)

$p4/mmm$ $4/mmm$ Tetragonal/Square

No. 61 $p4/m2/m2/m$ Patterson symmetry $p4/mmm$





Origin at centre $(4/mmm)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad x \le y; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2 \quad 0,0,z$
$(2_z|0,0,0)$

(3) $4^+ \quad 0,0,z$
$(4_z|0,0,0)$

(4) $4^- \quad 0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2 \quad 0,y,0$
$(2_y|0,0,0)$

(6) $2 \quad x,0,0$
$(2_x|0,0,0)$

(7) $2 \quad x,x,0$
$(2_{xy}|0,0,0)$

(8) $2 \quad x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

(9) $\bar{1} \quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $m \quad x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z|0,0,0)$

(12) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(13) $m \quad x,0,z$
$(m_y|0,0,0)$

(14) $m \quad 0,y,z$
$(m_x|0,0,0)$

(15) $m \quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(16) $m \quad x,x,z$
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) y,x,z	no conditions
							Special:
8	m	. m .	$x,\frac{1}{2},z$ $\bar{x},\frac{1}{2},\bar{z}$	$\bar{x},\frac{1}{2},z$ $x,\frac{1}{2},\bar{z}$	$\frac{1}{2},x,z$ $\frac{1}{2},x,\bar{z}$	$\frac{1}{2},\bar{x},z$ $\frac{1}{2},\bar{x},\bar{z}$	no extra conditions
8	l	. m .	$x,0,z$ $\bar{x},0,\bar{z}$	$\bar{x},0,z$ $x,0,\bar{z}$	$0,x,z$ $0,x,\bar{z}$	$0,\bar{x},z$ $0,\bar{x},\bar{z}$	no extra conditions
8	k	. . m	x,x,z $\bar{x},x,\bar{z}$	$\bar{x},\bar{x},z$ $x,\bar{x},\bar{z}$	$\bar{x},x,z$ $x,x,\bar{z}$	$x,\bar{x},z$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	j	m . .	$x,y,0$ $\bar{x},y,0$	$\bar{x},\bar{y},0$ $x,\bar{y},0$	$\bar{y},x,0$ $y,x,0$	$y,\bar{x},0$ $\bar{y},\bar{x},0$	no extra conditions
4	i	m 2m .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	h	m 2m .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	g	m . 2m	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	f	2 mm .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hk: $h+k=2n$
2	e	4 m m	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	d	4 m m	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	c	m mm .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk: $h+k=2n$
1	b	4/m m m	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	4/m m m	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I
[2] $p\bar{4}m2$ (59) 1; 2; 7; 8; 11; 12; 13; 14
[2] $p\bar{4}2m$ (57) 1; 2; 5; 6; 11; 12; 15; 16
[2] $p4mm$ (55) 1; 2; 3; 4; 13; 14; 15; 16
[2] $p422$ (53) 1; 2; 3; 4; 5; 6; 7; 8
[2] $p4/m11$ ($p4/m$, 51) 1; 2; 3; 4; 9; 10; 11; 12
[2] $p2/m12/m$ ($cmmm$, 47) 1; 2; 7; 8; 9; 10; 15; 16
[2] $p2/m2/m1$ ($pmmm$, 37) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $c4/amm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/nmm$, 64); [2] $c4/mmd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/mbm$, 63); [2] $c4/amd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/nbm$, 62)

Maximal isotypic subgroups of lowest index

IIc [2] $c4/mmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/mmm$, 61)

Minimal non-isotypic supergroups

I none

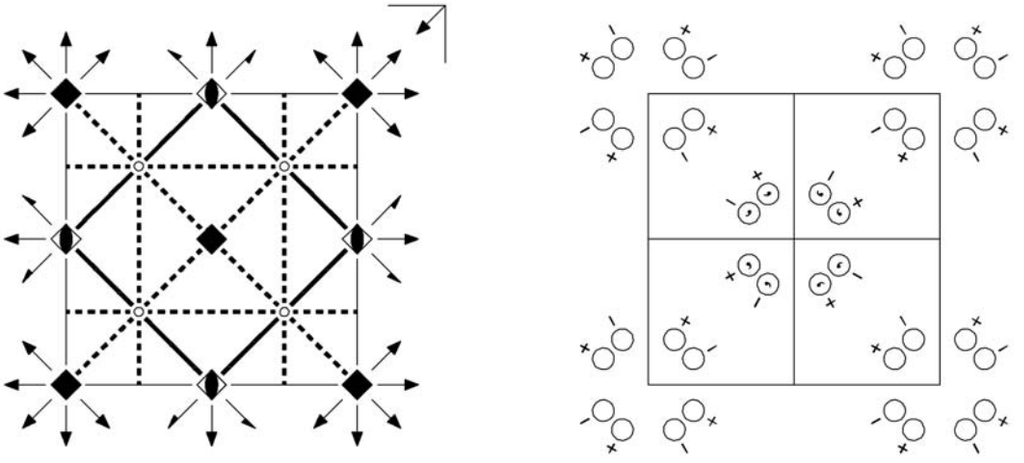
II none

International Tables for Crystallography (2010). Vol. E, Layer group 62, pp. 350–353.

$p4/nbm$ $4/mmm$ Tetragonal/Square

No. 62 $p4/n2/b2/m$ Patterson symmetry $p4/mmm$

ORIGIN CHOICE 1



Origin at 422 at $4/n22/g$ at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad y \le \frac{1}{2} - x; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) 2 $0,y,0$
$(2_y|0,0,0)$

(6) 2 $x,0,0$
$(2_x|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
$(\bar{1}|\frac{1}{2},\frac{1}{2},0)$

(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(11) $\bar{4}^+$ $\frac{1}{2},0,z;$ $\frac{1}{2},0,0$
$(\bar{4}_z|\frac{1}{2},\frac{1}{2},0)$

(12) $\bar{4}^-$ $\frac{1}{2},0,z;$ $\frac{1}{2},0,0$
$(\bar{4}_z^{-1}|\frac{1}{2},\frac{1}{2},0)$

(13) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(14) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

(15) m $x+\frac{1}{2},\bar{x},z$
$(m_{xy}|\frac{1}{2},\frac{1}{2},0)$

(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
$(m_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$ (9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$ (11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	hk: $h+k=2n$ $0k$: $k=2n$ $h0$: $h=2n$
							Special: as above, plus
8	h	. . m	$x,x+\frac{1}{2},z$ $\bar{x},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x,\bar{x}+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},x,z$ $x+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	no extra conditions
8	g	. 2 .	$x,0,0$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},0,0$ $x+\frac{1}{2},\frac{1}{2},0$	$0,x,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$	$0,\bar{x},0$ $\frac{1}{2},x+\frac{1}{2},0$	no extra conditions
8	f	. . 2	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},0$	$\bar{x},x,0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x,\bar{x},0$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	no extra conditions
4	e	2 . mm	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4	d	4 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	no extra conditions
4	c	. . $2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hk: $h,k=2n$
2	b	$\bar{4}$ 2 m	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			no extra conditions
2	a	4 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $\not/2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not/2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I
[2] $p\bar{4}b2$ (60) 1; 2; 7; 8; 11; 12; 13; 14
[2] $p\bar{4}2m$ (57) 1; 2; 5; 6; 11; 12; 15; 16
[2] $p4bm$ (56) 1; 2; 3; 4; 13; 14; 15; 16
[2] $p422$ (53) 1; 2; 3; 4; 5; 6; 7; 8
[2] $p4/n11$ ($p4/n$, 52) 1; 2; 3; 4; 9; 10; 11; 12
[2] $p2/n12/m$ ($cmme$, 48) 1; 2; 7; 8; 9; 10; 15; 16
[2] $p2/n2/b1$ ($pban$, 39) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (62)

Minimal non-isotypic supergroups

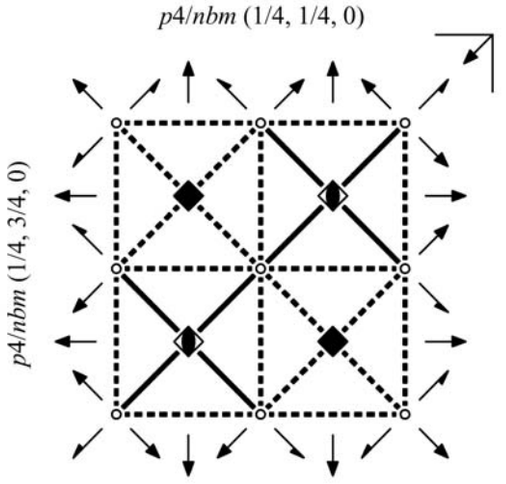
I none

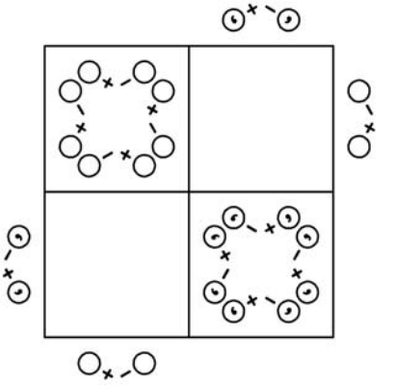
II [2] $c4/mmm$ ($p4/mmm$, 61)

$p4/nbm$ $(\frac{1}{4},\frac{1}{4},0)$ $4/mmm$ Tetragonal/Square

No. 62 $p4/n2/b2/m$ Patterson symmetry $p4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n(\mathbf{b},\mathbf{a})(2_1/g,2/m)$ at $\frac{1}{4},\frac{1}{4},0$ from 422

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad x\le -y;\quad 0\le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) $2\quad \frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(3) $4^+\quad \frac{1}{4},\frac{1}{4},z$
$(4_z|\frac{1}{2},0,0)$

(4) $4^-\quad \frac{1}{4},\frac{1}{4},z$
$(4_z^{-1}|0,\frac{1}{2},0)$

(5) $2\quad \frac{1}{4},y,0$
$(2_y|\frac{1}{2},0,0)$

(6) $2\quad x,\frac{1}{4},0$
$(2_x|0,\frac{1}{2},0)$

(7) $2\quad x,x,0$
$(2_{xy}|0,0,0)$

(8) $2\quad x,\bar{x}+\frac{1}{2},0$
$(2_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

(9) $\bar{1}\quad 0,0,0$
$(\bar{1}|0,0,0)$

(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(11) $\bar{4}^+\quad \frac{1}{4},-\frac{1}{4},z;\quad \frac{1}{4},-\frac{1}{4},0$
$(\bar{4}_z|\frac{1}{2},0,0)$

(12) $\bar{4}^-\quad -\frac{1}{4},\frac{1}{4},z;\quad -\frac{1}{4},\frac{1}{4},0$
$(\bar{4}_z^{-1}|0,\frac{1}{2},0)$

(13) $a\quad x,0,z$
$(m_y|\frac{1}{2},0,0)$

(14) $b\quad 0,y,z$
$(m_x|0,\frac{1}{2},0)$

(15) $m\quad x,\bar{x},z$
$(m_{xy}|0,0,0)$

(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$
$(m_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	hk: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	$h0$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	h	. . m	$x,\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z$	$x+\frac{1}{2},x,z$	$\bar{x},\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},x,\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	g	. 2 .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\frac{1}{4},x,0$	$\frac{1}{4},\bar{x}+\frac{1}{2},0$	no extra conditions
			$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	$\frac{3}{4},\bar{x},0$	$\frac{3}{4},x+\frac{1}{2},0$	
8	f	. . 2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	no extra conditions
			$\bar{x},\bar{x},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x},x+\frac{1}{2},0$	
4	e	2 . mm	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	no extra conditions
4	d	4 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	no extra conditions
4	c	. . 2/m	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	b	$\bar{4}$ 2 m	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			no extra conditions
2	a	4 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $\not|\, 2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not|\, 2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{4}b2$ (60) 1; 2; 7; 8; 11; 12; 13; 14
[2] $p\bar{4}2m$ (57) 1; 2; 5; 6; 11; 12; 15; 16
[2] $p4bm$ (56) 1; 2; 3; 4; 13; 14; 15; 16
[2] $p422$ (53) 1; 2; 3; 4; 5; 6; 7; 8
[2] $p4/n11$ ($p4/n$, 52) 1; 2; 3; 4; 9; 10; 11; 12
[2] $p2/n12/m$ ($cmme$, 48) 1; 2; 7; 8; 9; 10; 15; 16
[2] $p2/n2/b1$ ($pban$, 39) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (62)

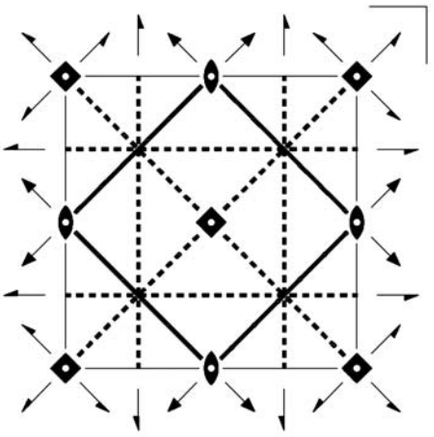
Minimal non-isotypic supergroups

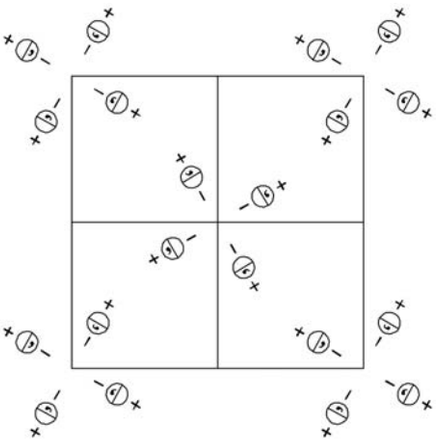
I none

II [2] $c4/mmm$ ($p4/mmm$, 61)

$p4/mbm$ $4/mmm$ Tetragonal/Square

No. 63 $p4/m2_1/b2/m$ Patterson symmetry $p4/mmm$





Origin at centre $(4/m)$ at $4/m12_1/g$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad y \le \frac{1}{2} - x; \quad 0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
$(2_x|\frac{1}{2},\frac{1}{2},0)$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
$(2_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) 2 $x,\bar{x}+\frac{1}{2},0$
$(2_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

(9) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(10) m $x,y,0$
$(m_z|0,0,0)$

(11) $\bar{4}^+$ $0,0,z;$ $0,0,0$
$(\bar{4}_z|0,0,0)$

(12) $\bar{4}^-$ $0,0,z;$ $0,0,0$
$(\bar{4}_z^{-1}|0,0,0)$

(13) a $x,\frac{1}{4},z$
$(m_y|\frac{1}{2},\frac{1}{2},0)$

(14) b $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},\frac{1}{2},0)$

(15) m $x+\frac{1}{2},\bar{x},z$
$(m_{xy}|\frac{1}{2},\frac{1}{2},0)$

(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
$(m_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$h0$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	g	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	f	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	e	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	d	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hk: $h+k=2n$
4	c	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hk: $h+k=2n$
2	b	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk: $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk: $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I
[2] $p\bar{4}b2$ (60) 1; 2; 7; 8; 11; 12; 13; 14
[2] $p\bar{4}2_1m$ (58) 1; 2; 5; 6; 11; 12; 15; 16
[2] $p4bm$ (56) 1; 2; 3; 4; 13; 14; 15; 16
[2] $p42_12$ (54) 1; 2; 3; 4; 5; 6; 7; 8
[2] $p4/m11$ ($p4/m$, 51) 1; 2; 3; 4; 9; 10; 11; 12
[2] $p2/m12/m$ ($cmmm$, 47) 1; 2; 7; 8; 9; 10; 15; 16
[2] $p2/m2_1/b1$ ($pbam$, 44) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/mbm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (63)

Minimal non-isotypic supergroups

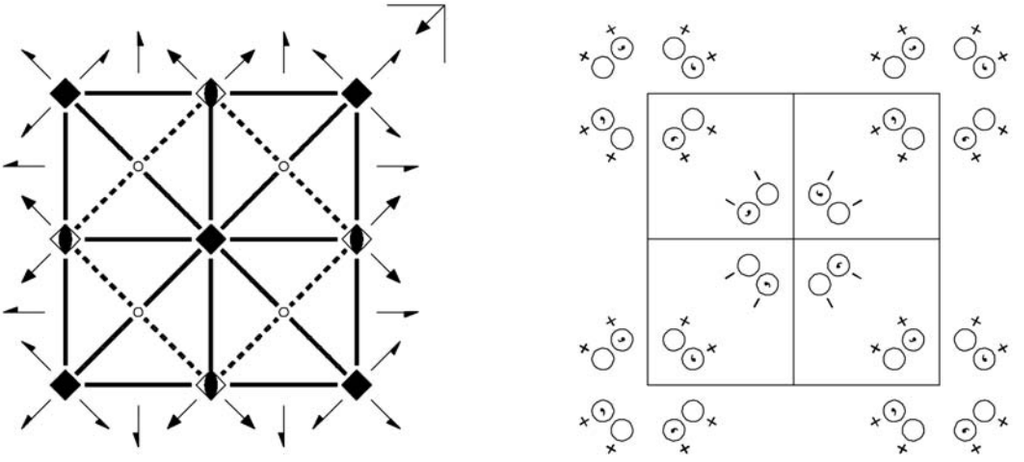
I none

II [2] $c4/mmm$ ($p4/mmm$, 61)

$p4/nmm$ $4/mmm$ Tetragonal/Square

No. 64 $p4/n2_1/m2/m$ Patterson symmetry $p4/mmm$

ORIGIN CHOICE 1



Origin on $4mm$ at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $y \le \frac{1}{2}-x$; $0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $0,0,z$
$(2_z|0,0,0)$

(3) 4^+ $0,0,z$
$(4_z|0,0,0)$

(4) 4^- $0,0,z$
$(4_z^{-1}|0,0,0)$

(5) $2(\frac{1}{2},\frac{1}{2},0)$ $0,y,0$
$(2_y|\frac{1}{2},\frac{1}{2},0)$

(6) $2(\frac{1}{2},\frac{1}{2},0)$ $x,0,0$
$(2_x|\frac{1}{2},\frac{1}{2},0)$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
$(2_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) $2(\frac{1}{2},\frac{1}{2},0)$ $x,\bar{x},0$
$(2_{\bar{x}y}|\frac{1}{2},\frac{1}{2},0)$

(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
$(\bar{1}|\frac{1}{2},\frac{1}{2},0)$

(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$
$(\bar{4}_z|\frac{1}{2},\frac{1}{2},0)$

(12) $\bar{4}^-$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$
$(\bar{4}_z^{-1}|\frac{1}{2},\frac{1}{2},0)$

(13) m $x,0,z$
$(m_y|0,0,0)$

(14) m $0,y,z$
$(m_x|0,0,0)$

(15) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(16) m x,x,z
$(m_{\bar{x}y}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hk: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h0$: $h=2n$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	g	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	f	$.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z$	$y,0,z$	no extra conditions
			$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$y+\frac{1}{2},\frac{1}{2},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}$	
8	e	$..2$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},0$	$x+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	$\bar{x},x+\frac{1}{2},0$	
4	d	$2\,mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4	c	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hk: $h,k=2n$
2	b	$4\,m\,m$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	a	$\bar{4}\,m\,2$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I	[2] $p\bar{4}m2$ (59)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $p\bar{4}2_1m$ (58)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4mm$ (55)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p42_12$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $p4/n11$ ($p4/n$, 52)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $p2/n12/m$ ($cmme$, 48)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $p2/n2_1/m1$ ($pmmn$, 46)	1; 2; 5; 6; 9; 10; 13; 14
IIa	none	
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (64)

Minimal non-isotypic supergroups

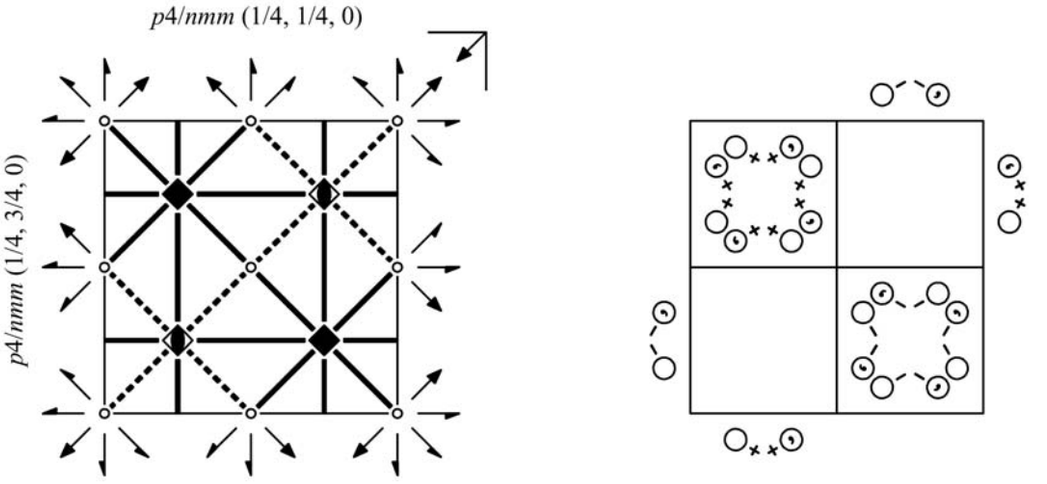
I none

II [2] $c4/mmm$ ($p4/mmm$, 61)

No. 64 $p4/n2_1/m2/m$

Patterson symmetry $p4/mmm$

ORIGIN CHOICE 2



Origin at centre $(2/m)$ at $n2_1(2/m,2_1/g)$ at $\frac{1}{4},\frac{1}{4},0$ from $4mm$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $x \le y$; $0 \le z$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 2 $\frac{1}{4},\frac{1}{4},z$
$(2_z|\frac{1}{2},\frac{1}{2},0)$

(3) 4^+ $\frac{1}{4},\frac{1}{4},z$
$(4_z|\frac{1}{2},0,0)$

(4) 4^- $\frac{1}{4},\frac{1}{4},z$
$(4_z^{-1}|0,\frac{1}{2},0)$

(5) $2(0,\frac{1}{2},0)$ $0,y,0$
$(2_y|0,\frac{1}{2},0)$

(6) $2(\frac{1}{2},0,0)$ $x,0,0$
$(2_x|\frac{1}{2},0,0)$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
$(2_{xy}|\frac{1}{2},\frac{1}{2},0)$

(8) 2 $x,\bar{x},0$
$(2_{\bar{x}y}|0,0,0)$

(9) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
$(m_z|\frac{1}{2},\frac{1}{2},0)$

(11) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$
$(\bar{4}_z|\frac{1}{2},0,0)$

(12) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
$(\bar{4}_z^{-1}|0,\frac{1}{2},0)$

(13) m $x,\frac{1}{4},z$
$(m_y|0,\frac{1}{2},0)$

(14) m $\frac{1}{4},y,z$
$(m_x|\frac{1}{2},0,0)$

(15) m $x+\frac{1}{2},\bar{x},z$
$(m_{xy}|\frac{1}{2},\frac{1}{2},0)$

(16) m x,x,z
$(m_{\bar{x}y}|0,0,0)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	hk: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0k$: $k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	$h0$: $h=2n$
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z	
							Special: as above, plus
8	g	$..m$	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x,\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	f	$.m.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\bar{y}+\frac{1}{2},\frac{1}{4},z$	$y,\frac{1}{4},z$	no extra conditions
			$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	$y+\frac{1}{2},\frac{3}{4},\bar{z}$	$\bar{y},\frac{3}{4},\bar{z}$	
8	e	$..2$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},x,0$	$\bar{x},\bar{x}+\frac{1}{2},0$	no extra conditions
			$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x},0$	$x,x+\frac{1}{2},0$	
4	d	$2\,mm.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	no extra conditions
4	c	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	b	$4\,m\,m$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	a	$\bar{4}\,m\,2$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I
[2] $p\bar{4}m2$ (59) 1; 2; 7; 8; 11; 12; 13; 14
[2] $p\bar{4}2_1m$ (58) 1; 2; 5; 6; 11; 12; 15; 16
[2] $p4mm$ (55) 1; 2; 3; 4; 13; 14; 15; 16
[2] $p42_12$ (54) 1; 2; 3; 4; 5; 6; 7; 8
[2] $p4/n11$ ($p4/n$, 52) 1; 2; 3; 4; 9; 10; 11; 12
[2] $p2/n12/m$ ($cmme$, 48) 1; 2; 7; 8; 9; 10; 15; 16
[2] $p2/n2_1/m1$ ($pmmn$, 46) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nmm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (64)

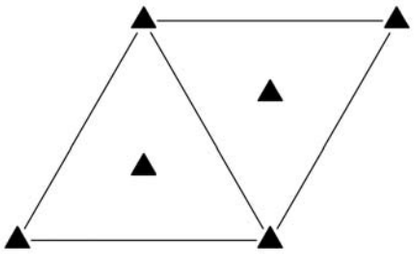
Minimal non-isotypic supergroups

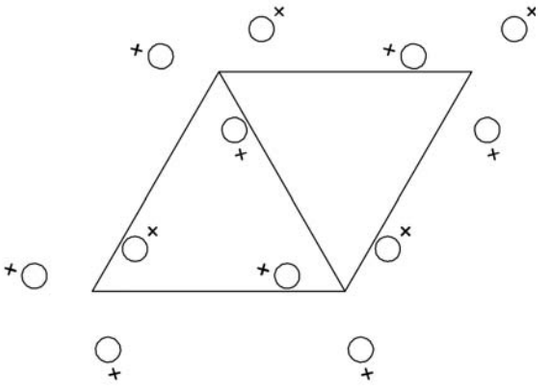
I none

II [2] $c4/mmm$ ($p4/mmm$, 61)

$p\,3$ 3 Trigonal/Hexagonal

No. 65 $p\,3$ Patterson symmetry $p\,\bar{3}$





Origin on 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1 (1|0,0,0)

(2) 3^+ 0,0,z (3_z|0,0,0)

(3) 3^- 0,0,z (3_z^{-1}|0,0,0)

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
						Special: no extra conditions
1	c	3 . .	$\frac{2}{3},\frac{1}{3},z$			
1	b	3 . .	$\frac{1}{3},\frac{2}{3},z$			
1	a	3 . .	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{m}1\,1\,1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{m}1\,1\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [3] $p1$ (1) 1
IIa none
IIb none

Maximal isotypic subgroups of lowest index

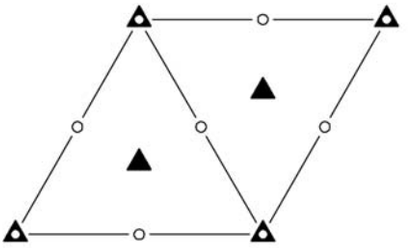
IIc [3] $h3$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p3$, 65)

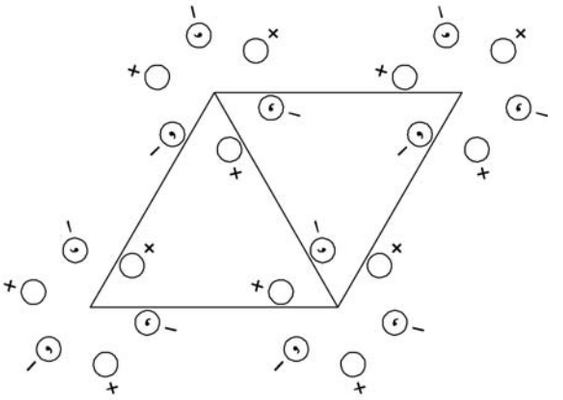
Minimal non-isotypic supergroups

I [2] $p\bar{3}$ (66); [2] $p312$ (67); [2] $p321$ (68); [2] $p3m1$ (69); [2] $p31m$ (70); [2] $p6$ (73); [2] $p\bar{6}$ (74)
II none

$p\bar{3}$ $\bar{3}$ Trigonal/Hexagonal

No. 66 $p\bar{3}$ Patterson symmetry $p\bar{3}$





Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(5) $\bar{3}^+$ $0,0,z$; $0,0,0$
$(\bar{3}_z|0,0,0)$

(6) $\bar{3}^-$ $0,0,z$; $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	e	1	(1) x,y,z (4) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,\bar{z}$	no conditions
						Special: no extra conditions
3	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	c	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	b	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	a	$\bar{3}$ . .	$0,0,0$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}211$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}211$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p3$ (65) 1; 2; 3
[3] $p\bar{1}$ (2) 1; 4

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\bar{3}$, 66)

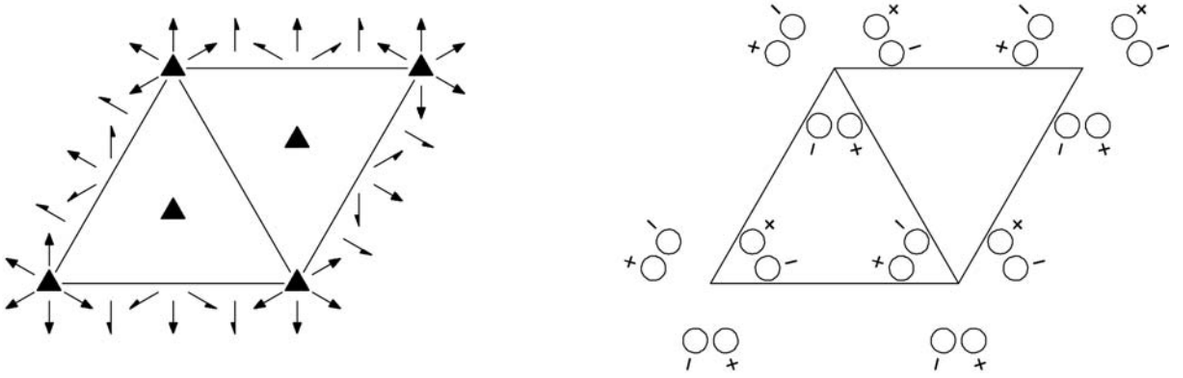
Minimal non-isotypic supergroups

I [2] $p\bar{3}1m$ (71); [2] $p\bar{3}m1$ (72); [2] $p6/m$ (75)

II none

$p312$ 312 Trigonal/Hexagonal

No. 67 $p312$ Patterson symmetry $p\bar{3}1m$



Origin at 312

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(5) 2 $x,2x,0$
$(2_2|0,0,0)$

(6) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
6	h	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}$	General: no conditions
						Special: no extra conditions
3	g	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	f	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	d	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	c	3 . 2	$\frac{2}{3},\frac{1}{3},0$			
1	b	3 . 2	$\frac{1}{3},\frac{2}{3},0$			
1	a	3 . 2	$0,0,0$			

Symmetry of special projections

Along [001] $p\,3\,m\,1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p\,2\,1\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\,3\,1\,1$ $(p\,3,\,65)$ 1; 2; 3
[3] $p\,1\,1\,2$ $(c\,2\,1\,1,\,10)$ 1; 4
[3] $p\,1\,1\,2$ $(c\,2\,1\,1,\,10)$ 1; 5
[3] $p\,1\,1\,2$ $(c\,2\,1\,1,\,10)$ 1; 6

IIa none

IIb [3] $h\,3\,1\,2$ $(\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b})$ $(p\,3\,2\,1,\,68)$

Maximal isotypic subgroups of lowest index

IIc [4] $p\,3\,1\,2$ $(\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b})$ (67)

Minimal non-isotypic supergroups

I [2] $p\,\bar{3}\,1\,m$ (71); [2] $p\,6\,2\,2$ (76); [2] $p\,\bar{6}\,m\,2$ (78)

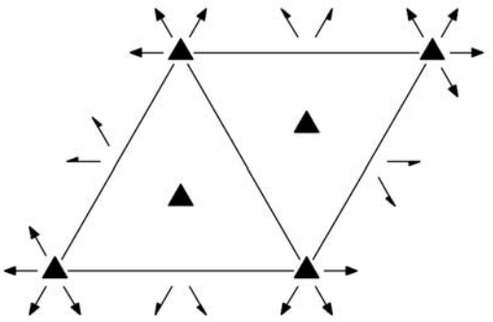
II [2] $h\,3\,1\,2$ $(p\,3\,2\,1,\,68)$

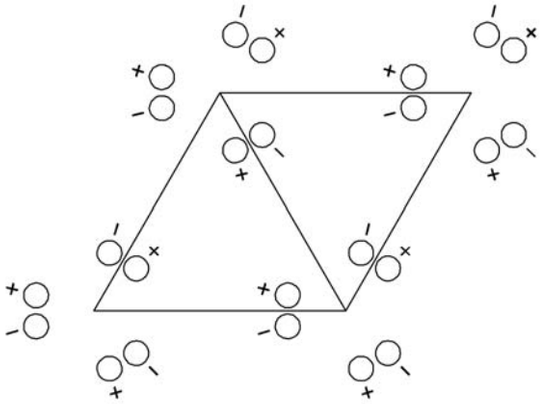
International Tables for Crystallography (2010). Vol. E, Layer group 68, pp. 366–367.

$p321$ 321 Trigonal/Hexagonal

No. 68 $p321$

Patterson symmetry $p\bar{3}m1$





Origin at 321

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(5) 2 $x,0,0$
$(2_x|0,0,0)$

(6) 2 $0,y,0$
$(2_y|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	e	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$	no conditions
						Special: no extra conditions
3	d	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
2	c	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	b	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	a	3 2 .	$0,0,0$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p211$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p311$ ($p3$, 65) 1; 2; 3
[3] $p121$ ($c211$, 10) 1; 4
[3] $p121$ ($c211$, 10) 1; 5
[3] $p121$ ($c211$, 10) 1; 6

IIa none

IIb [3] $h321$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p312$, 67)

Maximal isotypic subgroups of lowest index

IIc [4] $p321$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (68)

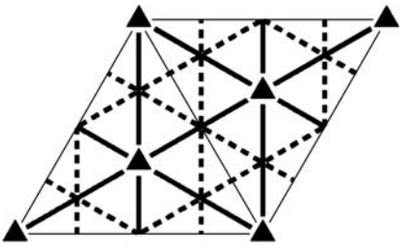
Minimal non-isotypic supergroups

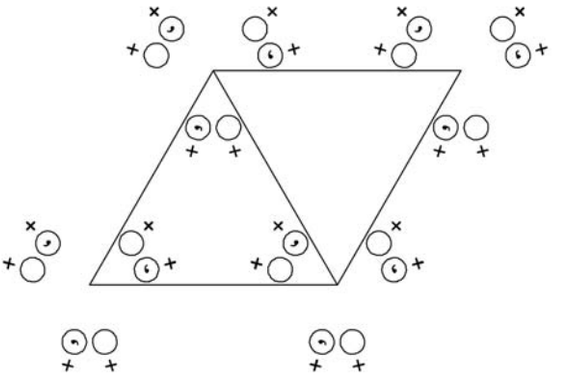
I [2] $p\bar{3}m1$ (72); [2] $p622$ (76); [2] $p\bar{6}2m$ (79)

II [2] $h321$ ($p312$, 67)

$p\,3\,m\,1$ $3\,m\,1$ Trigonal/Hexagonal

No. 69 $p\,3\,m\,1$ Patterson symmetry $p\,\bar{3}\,m\,1$





Origin on $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(5) m $x,2x,z$
$(m_x|0,0,0)$

(6) m $2x,x,z$
$(m_y|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
6	e	1	(1) x,y,z (4) $\bar{y},\bar{x},z$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,z$	General: no conditions
						Special: no extra conditions
3	d	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
1	c	3 m .	$\frac{2}{3},\frac{1}{3},z$			
1	b	3 m .	$\frac{1}{3},\frac{2}{3},z$			
1	a	3 m .	$0,0,z$			

Symmetry of special projections

Along [001] $p\,3\,m\,1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\,3\,1\,1$ ($p\,3$, 65) 1; 2; 3
[3] $p\,1\,m\,1$ ($c\,m\,1\,1$, 13) 1; 4
[3] $p\,1\,m\,1$ ($c\,m\,1\,1$, 13) 1; 5
[3] $p\,1\,m\,1$ ($c\,m\,1\,1$, 13) 1; 6

IIa none

IIb [3] $h\,3\,m\,1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\,3\,1\,m$, 70)

Maximal isotypic subgroups of lowest index

IIc [4] $p\,3\,m\,1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (69)

Minimal non-isotypic supergroups

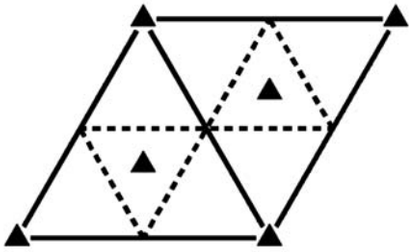
I [2] $p\,\bar{3}\,m\,1$ (72); [2] $p\,6\,m\,m$ (77); [2] $p\,\bar{6}\,m\,2$ (78)

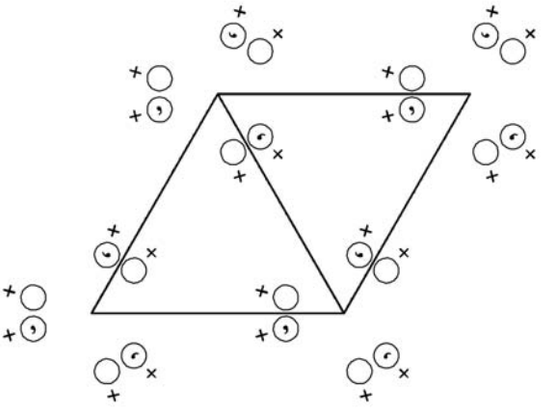
II [2] $h\,3\,m\,1$ ($p\,3\,1\,m$, 70)

International Tables for Crystallography (2010). Vol. E, Layer group 70, pp. 370–371.

$p\,3\,1\,m$ $3\,1\,m$ Trigonal/Hexagonal

No. 70 $p\,3\,1\,m$ Patterson symmetry $p\,\bar{3}\,1\,m$





Origin on $31m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 3^+ $0,0,z$ $(3_z|0,0,0)$

(3) 3^- $0,0,z$ $(3_z^{-1}|0,0,0)$

(4) m x,x,z $(m_3|0,0,0)$

(5) m $x,0,z$ $(m_2|0,0,0)$

(6) m $0,y,z$ $(m_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
6	d	1	(1) x,y,z (4) y,x,z	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,z$	General: no conditions
						Special: no extra conditions
3	c	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	
2	b	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	$3.m$	$0,0,z$			

Symmetry of special projections

Along [001] $p\,3\,1\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p\,1\,1\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\,3\,1\,1$ ($p\,3$, 65) 1; 2; 3
[3] $p\,1\,1\,m$ ($c\,m\,1\,1$, 13) 1; 4
[3] $p\,1\,1\,m$ ($c\,m\,1\,1$, 13) 1; 5
[3] $p\,1\,1\,m$ ($c\,m\,1\,1$, 13) 1; 6

IIa none

IIb [3] $h\,3\,1\,m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\,3\,m\,1$, 69)

Maximal isotypic subgroups of lowest index

IIc [4] $p\,3\,1\,m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (70)

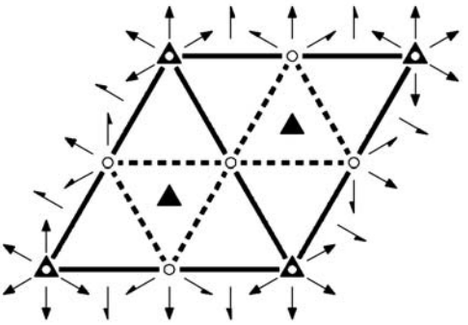
Minimal non-isotypic supergroups

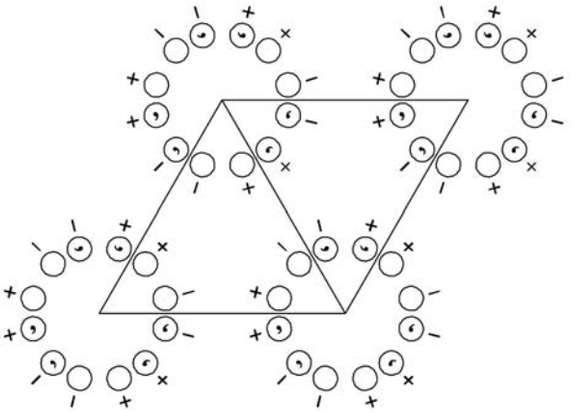
I [2] $p\,\bar{3}\,1\,m$ (71); [2] $p\,6\,m\,m$ (77); [2] $p\,\bar{6}\,2\,m$ (79)

II [2] $h\,3\,1\,m$ ($p\,3\,m\,1$, 69)

$p\bar{3}1m$ $\bar{3}1m$ Trigonal/Hexagonal

No. 71 $p\bar{3}12/m$ Patterson symmetry $p\bar{3}1m$





Origin at centre $(\bar{3}1m)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(5) 2 $x,2x,0$
$(2_2|0,0,0)$

(6) 2 $2x,x,0$
$(2_1|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	h	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) y,x,z	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x},\bar{x}+y,z$	no conditions
						Special: no extra conditions
6	g	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$0,\bar{x},\bar{z}$ $\bar{x},0,\bar{z}$ $x,x,\bar{z}$
6	f	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$ $\bar{x},2\bar{x},0$ $2x,x,0$
4	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$
3	d	. . 2/m	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	c	3 . m	$0,0,z$	$0,0,\bar{z}$		
2	b	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$		
1	a	$\bar{3}$. m	$0,0,0$			

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}211$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p31m$ (70) 1; 2; 3; 10; 11; 12
[2] $p312$ (67) 1; 2; 3; 4; 5; 6
[2] $p\bar{3}11$ ($p\bar{3}$, 66) 1; 2; 3; 7; 8; 9
[3] $p112/m$ ($c2/m11$, 18) 1; 4; 7; 10
[3] $p112/m$ ($c2/m11$, 18) 1; 5; 7; 11
[3] $p112/m$ ($c2/m11$, 18) 1; 6; 7; 12

IIa none

IIb [3] $h\bar{3}1m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\bar{3}m1$, 72)

Maximal isotypic subgroups of lowest index

IIc [4] $p\bar{3}1m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (71)

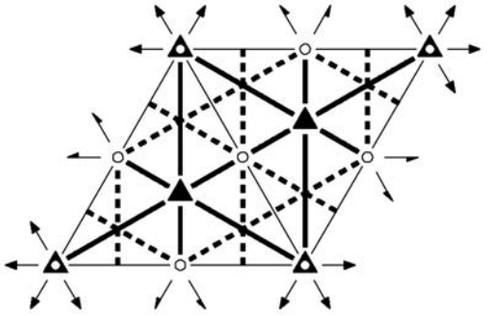
Minimal non-isotypic supergroups

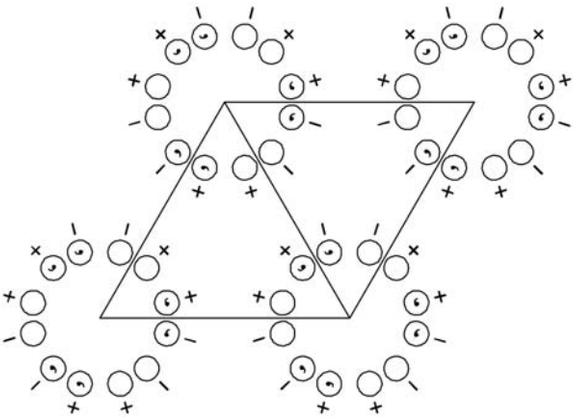
I [2] $p6/mmm$ (80)

II [2] $h\bar{3}1m$ ($p\bar{3}m1$, 72)

$p\bar{3}m1$ $\bar{3}m1$ Trigonal/Hexagonal

No. 72 $p\bar{3}2/m1$ Patterson symmetry $p\bar{3}m1$





Origin at centre $(\bar{3}m1)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(5) 2 $x,0,0$
$(2_x|0,0,0)$

(6) 2 $0,y,0$
$(2_y|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(11) m $x,2x,z$
$(m_x|0,0,0)$

(12) m $2x,x,z$
$(m_y|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$	
						Special: no extra conditions
6	f	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$ $2x,x,\bar{z}$ $\bar{x},2\bar{x},\bar{z}$
6	e	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$ $0,\bar{x},0$ $x,x,0$
3	d	. $2/m$.	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	c	3 m .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	b	3 m .	$0,0,z$	$0,0,\bar{z}$		
1	a	$\bar{3}$ m .	$0,0,0$			

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2\,1\,1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p3m1$ (69) 1; 2; 3; 10; 11; 12
[2] $p321$ (68) 1; 2; 3; 4; 5; 6
[2] $p\bar{3}11$ ($p\bar{3}$, 66) 1; 2; 3; 7; 8; 9
[3] $p12/m1$ ($c2/m11$, 18) 1; 4; 7; 10
[3] $p12/m1$ ($c2/m11$, 18) 1; 5; 7; 11
[3] $p12/m1$ ($c2/m11$, 18) 1; 6; 7; 12

IIa none

IIb [3] $h\bar{3}m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\bar{3}1m$, 71)

Maximal isotypic subgroups of lowest index

IIc [4] $p\bar{3}m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (72)

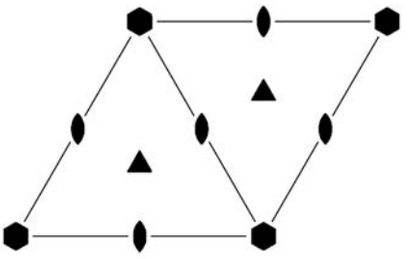
Minimal non-isotypic supergroups

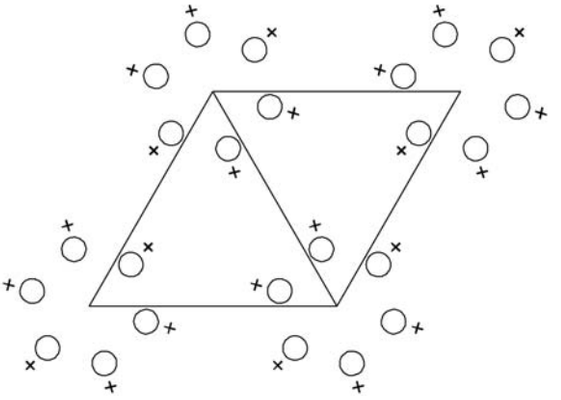
I [2] $p6/mmm$ (80)

II [2] $h\bar{3}m1$ ($p\bar{3}1m$, 71)

$p6$ 6 Hexagonal/Hexagonal

No. 73 $p6$ Patterson symmetry $p6/m$





Origin on 6

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
6	d	1	(1) x,y,z (4) $\bar{x},\bar{y},z$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$	General: no conditions
						Special: no extra conditions
3	c	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	
2	b	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	6 . .	$0,0,z$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p3$ (65) 1; 2; 3
[3] $p211$ ($p112$, 3) 1; 4

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h6$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p6$, 73)

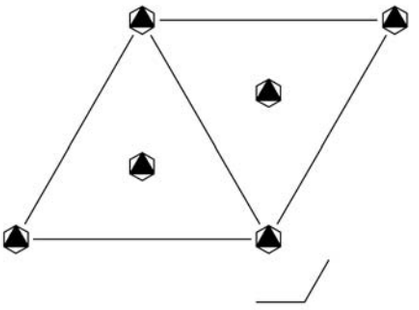
Minimal non-isotypic supergroups

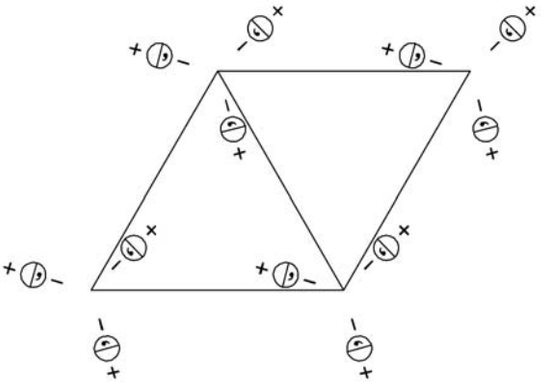
I [2] $p6/m$ (75); [2] $p622$ (76); [2] $p6mm$ (77)

II none

$p\bar{6}$ $\bar{6}$ Hexagonal/Hexagonal

No. 74 $p\bar{6}$ Patterson symmetry $p6/m$





Origin at $\bar{6}$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z$; $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
$(\bar{6}_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	h	1	(1) x,y,z (4) $x,y,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$	no conditions
						Special: no extra conditions
3	g	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	
2	f	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	d	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	c	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},0$			
1	b	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$			
1	a	$\bar{6}$ . .	$0,0,0$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p3$ (65) 1; 2; 3
[3] $pm11$ ($p11m$, 4) 1; 4

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h\bar{6}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p\bar{6}$, 74)

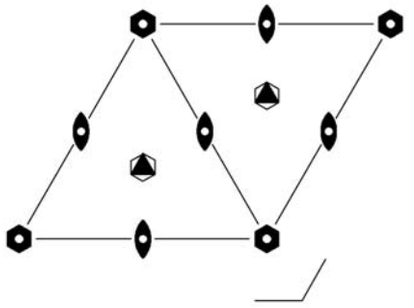
Minimal non-isotypic supergroups

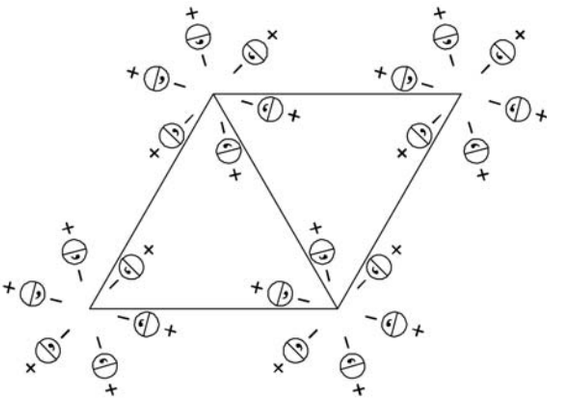
I [2] $p6/m$ (75); [2] $p\bar{6}m2$ (78); [2] $p\bar{6}2m$ (79)

II none

$p6/m$ $6/m$ Hexagonal/Hexagonal

No. 75 $p6/m$ Patterson symmetry $p6/m$





Origin at centre $(6/m)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) $\bar{1}$ $0,0,0$
$(\bar{1}|0,0,0)$

(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
$(\bar{3}_z|0,0,0)$

(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
$(\bar{3}_z^{-1}|0,0,0)$

(10) m $x,y,0$
$(m_z|0,0,0)$

(11) $\bar{6}^-$ $0,0,z$; $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(12) $\bar{6}^+$ $0,0,z$; $0,0,0$
$(\bar{6}_z|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	h	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{y},x-y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $x-y,x,\bar{z}$ (12) $\bar{x}+y,\bar{x},\bar{z}$	no conditions
						Special: no extra conditions
6	g	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$ $y,\bar{x}+y,0$ $x-y,x,0$
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},\bar{z}$ $\frac{1}{2},\frac{1}{2},\bar{z}$
4	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$
3	d	$2/m$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	c	6 . .	$0,0,z$	$0,0,\bar{z}$		
2	b	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$		
1	a	$6/m$ . .	$0,0,0$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{6}$ (74) 1; 2; 3; 10; 11; 12
[2] $p6$ (73) 1; 2; 3; 4; 5; 6
[2] $p\bar{3}$ (66) 1; 2; 3; 7; 8; 9
[3] $p2/m11$ ($p112/m$, 6) 1; 4; 7; 10

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h6/m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p6/m$, 75)

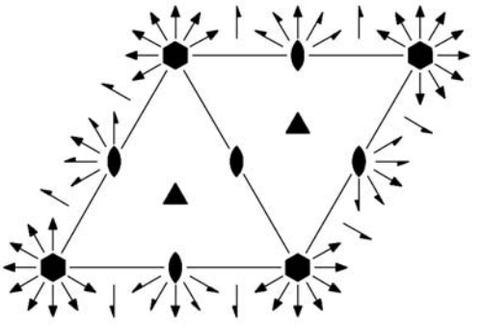
Minimal non-isotypic supergroups

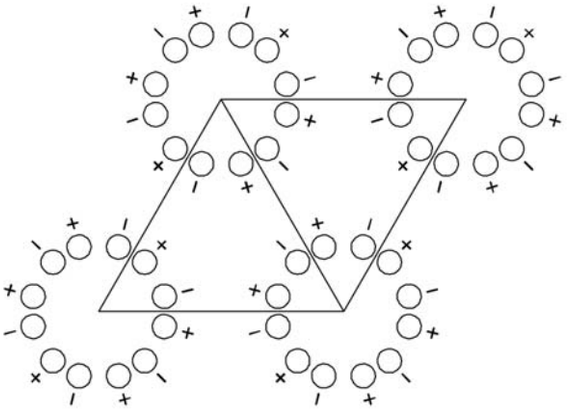
I [2] $p6/mmm$ (80)

II none

$p622$ 622 Hexagonal/Hexagonal

No. 76 $p622$ Patterson symmetry $p6/mmm$





Origin at 622

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}$				no conditions
									Special: no extra conditions
6	h	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
6	g	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	
4	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			
3	d	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	c	6 . .	$0,0,z$	$0,0,\bar{z}$					
2	b	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	a	6 2 2	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p611$ ($p6$, 73) 1; 2; 3; 4; 5; 6
[2] $p321$ (68) 1; 2; 3; 7; 8; 9
[2] $p312$ (67) 1; 2; 3; 10; 11; 12
[3] $p222$ ($c222$, 22) 1; 4; 7; 10
[3] $p222$ ($c222$, 22) 1; 4; 8; 11
[3] $p222$ ($c222$, 22) 1; 4; 9; 12

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h622$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p622$, 76)

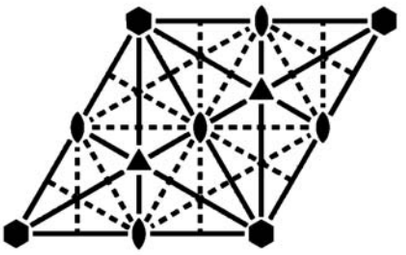
Minimal non-isotypic supergroups

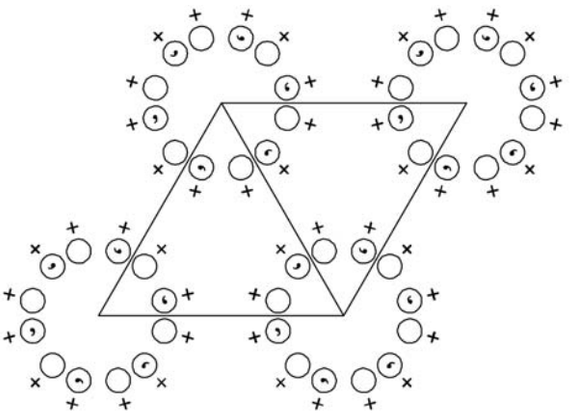
I [2] $p6/mmm$ (80)

II none

$p6mm$ $6mm$ Hexagonal/Hexagonal

No. 77 $p6mm$ Patterson symmetry $p6/mmm$





Origin on $6mm$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$
$(2_z|0,0,0)$

(5) 6^- $0,0,z$
$(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$
$(6_z|0,0,0)$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m $x,2x,z$
$(m_x|0,0,0)$

(9) m $2x,x,z$
$(m_y|0,0,0)$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $\bar{y},\bar{x},z$ (10) y,x,z	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $\bar{x}+y,y,z$ (11) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $x,x-y,z$ (12) $\bar{x},\bar{x}+y,z$	no conditions
						Special: no extra conditions
6	e	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z$	$\bar{x},2\bar{x},z$	$2x,x,z$
6	d	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$	$0,\bar{x},z$	x,x,z
3	c	2 m m	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$			
2	b	3 m .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$				
1	a	6 m m	$0,0,z$					

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $\not\!/1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not\!/1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I
[2] $p6\,1\,1$ ($p6$, 73) 1; 2; 3; 4; 5; 6
[2] $p3\,1\,m$ (70) 1; 2; 3; 10; 11; 12
[2] $p3\,m\,1$ (69) 1; 2; 3; 7; 8; 9
[3] $p2mm$ ($cmm2$, 26) 1; 4; 7; 10
[3] $p2mm$ ($cmm2$, 26) 1; 4; 8; 11
[3] $p2mm$ ($cmm2$, 26) 1; 4; 9; 12

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [3] $h6mm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p6mm$, 77)

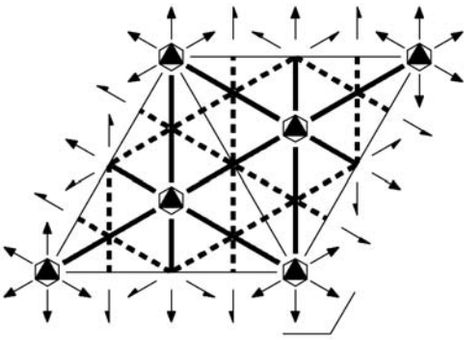
Minimal non-isotypic supergroups

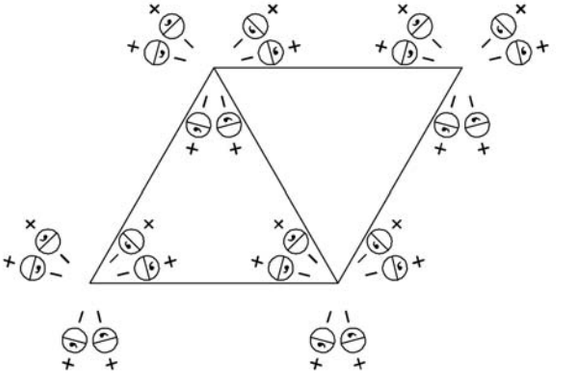
I [2] $p6/mmm$ (80)

II none

$p\bar{6}m2$ $\bar{6}m2$ Hexagonal/Hexagonal

No. 78 $p\bar{6}m2$ Patterson symmetry $p6/mmm$





Origin at $\bar{6}m2$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le 2y$; $y \le \min(1-x, 2x)$; $0 \le z$

Vertices $0,0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z$; $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) m $x,\bar{x},z$
$(m_{xy}|0,0,0)$

(8) m $x,2x,z$
$(m_x|0,0,0)$

(9) m $2x,x,z$
$(m_y|0,0,0)$

(10) 2 $x,\bar{x},0$
$(2_3|0,0,0)$

(11) 2 $x,2x,0$
$(2_2|0,0,0)$

(12) 2 $2x,x,0$
$(2_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	j	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$	
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$	
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$	
						Special: no extra conditions
6	i	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$ $x,2x,\bar{z}$ $2\bar{x},\bar{x},\bar{z}$
6	h	$m..$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{y},\bar{x},0$ $\bar{x}+y,y,0$ $x,x-y,0$
3	g	$mm2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	f	$3m.$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	e	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	d	$3m.$	$0,0,z$	$0,0,\bar{z}$		
1	c	$\bar{6}m2$	$\frac{2}{3},\frac{1}{3},0$			
1	b	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},0$			
1	a	$\bar{6}m2$	$0,0,0$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{6}11$ ($p\bar{6}$, 74) 1; 2; 3; 4; 5; 6
[2] $p3m1$ (69) 1; 2; 3; 7; 8; 9
[2] $p312$ (67) 1; 2; 3; 10; 11; 12
[3] $pmm2$ ($cm2m$, 35) 1; 4; 7; 10
[3] $pmm2$ ($cm2m$, 35) 1; 4; 8; 11
[3] $pmm2$ ($cm2m$, 35) 1; 4; 9; 12

IIa none

IIb [3] $h\bar{6}m2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p\bar{6}2m$, 79)

Maximal isotypic subgroups of lowest index

IIc [4] $p\bar{6}m2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (78)

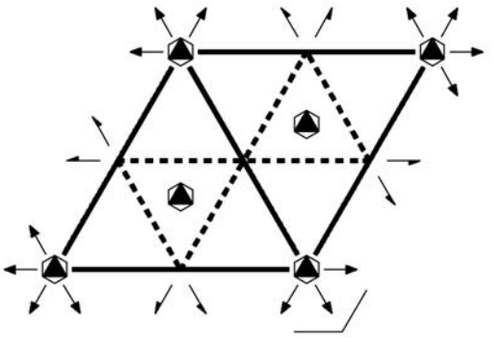
Minimal non-isotypic supergroups

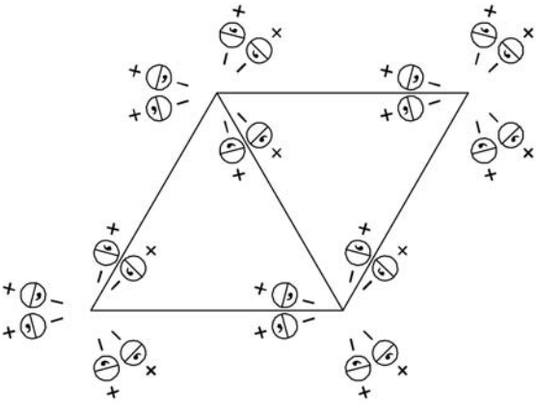
I [2] $p6/mmm$ (80)

II [2] $h\bar{6}m2$ ($p\bar{6}2m$, 79)

$p\bar{6}2m$ $\bar{6}2m$ Hexagonal/Hexagonal

No. 79 $p\bar{6}2m$ Patterson symmetry $p6/mmm$





Origin at $\bar{6}2m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
$(1|0,0,0)$

(2) 3^+ $0,0,z$
$(3_z|0,0,0)$

(3) 3^- $0,0,z$
$(3_z^{-1}|0,0,0)$

(4) m $x,y,0$
$(m_z|0,0,0)$

(5) $\bar{6}^-$ $0,0,z$; $0,0,0$
$(\bar{6}_z^{-1}|0,0,0)$

(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
$(\bar{6}_z|0,0,0)$

(7) 2 $x,x,0$
$(2_{xy}|0,0,0)$

(8) 2 $x,0,0$
$(2_x|0,0,0)$

(9) 2 $0,y,0$
$(2_y|0,0,0)$

(10) m x,x,z
$(m_3|0,0,0)$

(11) m $x,0,z$
$(m_2|0,0,0)$

(12) m $0,y,z$
$(m_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	h	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$	
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
6	g	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$y,x,0$ $x-y,\bar{y},0$ $\bar{x},\bar{x}+y,0$
6	f	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$x,0,\bar{z}$ $0,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$
4	e	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$
3	d	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
2	c	3 . m	$0,0,z$	$0,0,\bar{z}$		
2	b	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$		
1	a	$\bar{6}\,2\,m$	$0,0,0$			

Symmetry of special projections

Along [001] $p3\,1\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $\not{p}2\,m\,m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $\not{p}1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I [2] $p\bar{6}\,1\,1$ ($p\bar{6}$, 74) 1; 2; 3; 4; 5; 6
[2] $p3\,1\,m$ (70) 1; 2; 3; 10; 11; 12
[2] $p3\,2\,1$ (68) 1; 2; 3; 7; 8; 9
[3] $pm2m$ ($cm2m$, 35) 1; 4; 7; 10
[3] $pm2m$ ($cm2m$, 35) 1; 4; 8; 11
[3] $pm2m$ ($cm2m$, 35) 1; 4; 9; 12

IIa none

IIb [3] $h\bar{6}\,2\,m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p\bar{6}m2$, 78)

Maximal isotypic subgroups of lowest index

IIc [4] $p\bar{6}\,2\,m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (79)

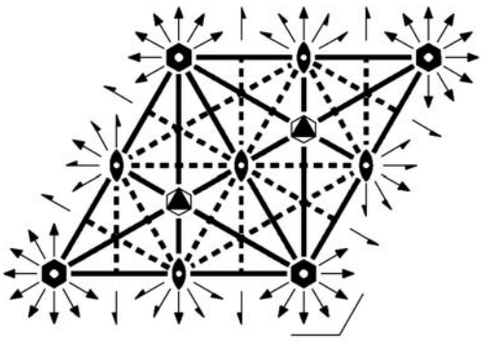
Minimal non-isotypic supergroups

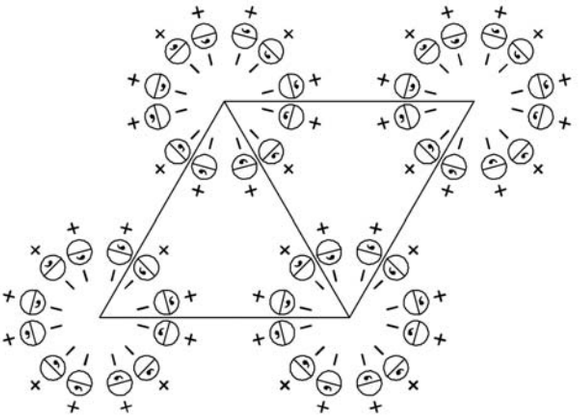
I [2] $p6/mmm$ (80)

II [2] $h\bar{6}\,2\,m$ ($p\bar{6}m2$, 78)

$p6/mmm$ $6/mmm$ Hexagonal/Hexagonal

No. 80 $p6/mmm$ Patterson symmetry $p6/mmm$





Origin at centre $(6/mmm)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le x/2$; $0 \le z$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) 3^+ $0,0,z$ $(3_z|0,0,0)$

(3) 3^- $0,0,z$ $(3_z^{-1}|0,0,0)$

(4) 2 $0,0,z$ $(2_z|0,0,0)$

(5) 6^- $0,0,z$ $(6_z^{-1}|0,0,0)$

(6) 6^+ $0,0,z$ $(6_z|0,0,0)$

(7) 2 $x,x,0$ $(2_{xy}|0,0,0)$

(8) 2 $x,0,0$ $(2_x|0,0,0)$

(9) 2 $0,y,0$ $(2_y|0,0,0)$

(10) 2 $x,\bar{x},0$ $(2_3|0,0,0)$

(11) 2 $x,2x,0$ $(2_2|0,0,0)$

(12) 2 $2x,x,0$ $(2_1|0,0,0)$

(13) $\bar{1}$ $0,0,0$ $(\bar{1}|0,0,0)$

(14) $\bar{3}^+$ $0,0,z$; $0,0,0$ $(\bar{3}_z|0,0,0)$

(15) $\bar{3}^-$ $0,0,z$; $0,0,0$ $(\bar{3}_z^{-1}|0,0,0)$

(16) m $x,y,0$ $(m_z|0,0,0)$

(17) $\bar{6}^-$ $0,0,z$; $0,0,0$ $(\bar{6}_z^{-1}|0,0,0)$

(18) $\bar{6}^+$ $0,0,z$; $0,0,0$ $(\bar{6}_z|0,0,0)$

(19) m $x,\bar{x},z$ $(m_{xy}|0,0,0)$

(20) m $x,2x,z$ $(m_x|0,0,0)$

(21) m $2x,x,z$ $(m_y|0,0,0)$

(22) m x,x,z $(m_3|0,0,0)$

(23) m $x,0,z$ $(m_2|0,0,0)$

(24) m $0,y,z$ $(m_1|0,0,0)$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	
			(16) $x,y,\bar{z}$	(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$	
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$	
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
12	k	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$
			$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	$\bar{y},\bar{x},0$	$\bar{x}+y,y,0$	$x,x-y,0$
12	j	. m .	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z$	$2x,x,z$	$\bar{x},x,z$
			$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}$	$x,2x,\bar{z}$	$x,\bar{x},\bar{z}$
12	i	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$	$0,\bar{x},z$	x,x,z
			$0,x,\bar{z}$	$x,0,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$
6	h	$m\,m\,2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$
6	g	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$
6	f	$2\,m\,m$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$
4	e	$3\,m$.	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
3	d	$m\,m\,m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	c	$6\,m\,m$	$0,0,z$	$0,0,\bar{z}$				
2	b	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$				
1	a	$6/m\,m\,m$	$0,0,0$					

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isotypic subgroups

I	[2] $p\bar{6}2m$ (79)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $p\bar{6}m2$ (78)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $p6mm$ (77)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $p622$ (76)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $p6/m11$ ($p6/m$, 75)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $p\bar{3}m1$ (72)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $p\bar{3}1m$ (71)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[3] $pmmm$ ($cmmm$, 47)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $pmmm$ ($cmmm$, 47)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $pmmm$ ($cmmm$, 47)	1; 4; 9; 12; 13; 16; 21; 24
IIa	none	
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [3] $h6/mmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p6/mmm$, 80)

Minimal non-isotypic supergroups

I none

II none

5.1. Symbols used in Parts 5 and 6

$\mathcal{G}$	Scanned space group
P	Origin of the coordinate system of the scanned space group $\mathcal{G}$
$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	Conventional basis vectors of the scanned space group $\mathcal{G}$
$(P; \mathbf{a}, \mathbf{b}, \mathbf{c})$	Conventional coordinate system of the scanned space group $\mathcal{G}$
(hkl)	Miller indices of a section plane
$(hkil)$	Bravais–Miller indices of a section plane
$(mn0)$	Miller indices for special orientations with variable parameter
$V(\mathbf{a}', \mathbf{b}')$	Orientation of planes defined by Miller or Miller–Bravais indices
$\mathcal{H}(\mathcal{G}, (hkl)) = \mathcal{H}(\mathcal{G}, V(\mathbf{a}', \mathbf{b}'))$	Scanning group for the scanned group $\mathcal{G}$ and orientation $V(\mathbf{a}', \mathbf{b}')$ defined by Miller indices (hkl)
$\mathcal{H}$	Shorthand notation for the scanning group
$\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$	Conventional basis vectors of the scanning group
$\mathbf{a}'$, $\mathbf{b}'$	Conventional basis vectors of the sectional layer groups for a given orientation of the section plane
$\mathbf{d}$	Basis vector of the scanning group in the scanning direction
$\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$	Auxiliary basis of a monoclinic scanning group
s	Distance of a section plane from the origin P in units of $\mathbf{d}$
$P + s\mathbf{d}$	Location of the section plane along the scanning line
$\mathcal{L}(P + s\mathbf{d}; (hkl))$	Sectional layer group of a plane with orientation (hkl) passing through the point $P + s\mathbf{d}$
$\mathcal{L}(s\mathbf{d})$	Shorthand notation for this sectional layer group
$(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$	Reference coordinate system for the sectional layer group
$s_o = 1/f$	Length of the fundamental region along $\mathbf{d}$ in units of $\mathbf{d}$
$f = 1/s_o$	Number of planes of a general translation orbit in the interval $0 \leq s < 1$
S_1, S_2	Single domain states
$(\mathsf{S}_1, \mathsf{S}_2)$	Ordered domain pair
$\{\mathsf{S}_1, \mathsf{S}_2\}$	Unordered domain pair
$\mathcal{F}_{12}$	Symmetry group of an ordered domain pair
$\mathcal{J}_{12}$	Symmetry group of an unordered domain pair
$(\mathsf{S}_1\|(hkl), s\mathbf{d}\|\mathsf{S}_2) = (\mathsf{S}_1\|\mathbf{n}, s\mathbf{d}\|\mathsf{S}_2)$	Domain twin with a central plane of orientation and sidedness defined by Miller indices (hkl) or by a normal $\mathbf{n}$, and location $s\mathbf{d}$
$\overline{\mathsf{F}}_{12}$, $\widehat{\mathsf{F}}_{12}$	Sectional layer group of the central plane under the action of the group $\mathcal{F}_{12}$ and its floating subgroup
$\overline{\mathsf{J}}_{12}$, $\widehat{\mathsf{J}}_{12}$	Sectional layer group of the central plane under the action of the group $\mathcal{J}_{12}$ and its floating subgroup
T_{12}	Symmetry group of the domain twin
f_{12}	Trivial symmetry operations of the twin
$\underline{t}^*_{12}$	Nontrivial symmetry operations of the twin
$\underline{s}_{12}$	Side-reversing operations of the twin
r^*_{12}	State-reversing operations of the twin

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5.2. Guide to the use of the scanning tables

5.2.1. Introduction

The global symmetry of an ideal crystal is described by its space group $\mathcal{G}$. It is also of interest to consider symmetries of local character. The classical example is that of the site symmetries, which are the symmetries of individual points in a crystal. These are completely described and classified as a part of the standard description of space groups in *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 2005). The results of this procedure contain two types of information:

(i) site symmetries of individual points under the action of the group $\mathcal{G}$ and

(ii) orbits of points under the action of the group $\mathcal{G}$.

This information, apart from its use, for example, in the consideration of the splitting of atomic levels in the field of the site symmetry, provides the background for the description of crystal structure: points of the same orbit are occupied by identical atoms (ions) and the environment of these atoms (ions) is also identical. A complete description of the structure is reduced to a description of the occupation of individual Wyckoff positions.

Analogously, we may consider the symmetries of planes transecting the crystal and of straight lines penetrating the crystal, called here the *sectional layer groups* (*symmetries*) and the *penetration rod groups* (*symmetries*). Here we look again for the two types of information:

(i) symmetries of individual planes (straight lines) under the action of the group $\mathcal{G}$ and

(ii) orbits of planes (straight lines) under the action of the group $\mathcal{G}$.

The general law that describes the connection between local symmetries and orbits of points, planes or straight lines is expressed by a coset resolution of the space group with respect to local symmetries. The orbits of planes (straight lines) have analogous properties to orbits of points. The structure of the plane (straight line) and its environment is identical for different planes (straight lines) of the same orbit. This is useful in the consideration of layer structures, see Section 5.2.5.1, and of structures with pronounced rod arrangements.

Layer symmetries have also been found to be indispensable in *bicrystallography*, see Section 5.2.5.2. This term and the term *bicrystal* were introduced by Pond & Bollmann (1979) with reference to the study of grain boundaries [see also Pond & Vlachavas (1983) and Vlachavas (1985)]. A bicrystal is in general an edifice where two crystals, usually of the same structure but of different orientations, meet at a common boundary – an interface. The sectional layer groups are appropriate for both the description of symmetries of such boundary planes and the description of the bicrystals.

The *sectional layer groups* were, however, introduced much earlier by Holser (1958*a*,*b*) in connection with the consideration of domain walls and twin boundaries as symmetry groups of planes bisecting the crystal. The mutual orientations of the two components of a bicrystal are in general arbitrary. In the case of domain walls and twin boundaries, which can be considered as interfaces of special types of bicrystals, there are crystallographic restrictions on these orientations. The group-theoretical basis for an analysis of domain pairs is given by Janovec (1972). The consideration of the structure of domain walls or twin boundaries involves the sectional layer groups (Janovec, 1981; Zikmund, 1984); they were examined in the particular cases of domain structure in KSCN crystals (Janovec *et al.*, 1989) and of domain walls and antiphase boundaries in calomel crystals (Janovec & Zikmund, 1993), see Section 5.2.5.3, and recently also in fullerene C_{60} (Janovec & Kopský, 1997; Saint-Grégoire *et al.*, 1997).

The first attempts to derive the sectional layer groups systematically were made by Wondratschek (1971) and by using a computer program written by Guigas (1971). Davies & Dirl (1993*a*) developed a program for finding subgroups of space groups, which they later modified to find sectional layer groups and penetration rod groups as well (Davies & Dirl, 1993*b*). The use and determination of sectional layer groups have also been discussed by Janovec *et al.* (1988), Kopský & Litvin (1989) and Fuksa *et al.* (1993).

The penetration rod groups can be used in the consideration of linear edifices in a crystal, *e.g.* line dislocations or intersections of boundaries, or in crystals with pronounced rod arrangements. So far, there seems to be no interest in the penetration rod groups and there is actually no need to produce special tables for these groups. Determining penetration rod groups was found to be a complementary problem to that of determining sectional layer groups (Kopský, 1989*c*, 1990).

The keyword for this part of this volume is the term *scanning*, introduced by Kopský (1990) for the description of the spatial distribution of local symmetries. In this sense, the description of site symmetries and classification of point orbits by Wyckoff positions are a result of the *scanning* of the space group for the site symmetries.

The *Scanning tables*, Part 6, give a complete set of information on the space distribution of sectional layer groups and of the penetration rod groups. They were derived using the *scanning-group* method and the *scanning theorem*, see Section 5.2.2.2. The tables describe explicitly the scanning for the sectional layer groups. The spatial distribution of (scanning for) the penetration rod groups is seen directly from the *scanning groups*, which are given as a part of the information in the scanning tables.

The sectional layer groups and the penetration rod groups are subgroups of space groups and as such act on the three-dimensional point space. The examples of particular studies in Section 5.2.5 emphasize the importance of the exact location of sectional layer groups with reference to the crystal structure and hence to the crystallographic coordinate system. In the usual interpretation, Hermann–Mauguin symbols do not specify the location of the group in space. In the scanning tables, each Hermann–Mauguin symbol means a quite specific space or layer group with reference to a specified crystallographic coordinate system, see Sections 5.2.3.1.1 and 5.2.3.1.4.

The layer and rod groups can also be interpreted as factor groups of reducible space groups (Kopský, 1986, 1988, 1989*a*,*b*, 1993*a*; Fuksa & Kopský, 1993). Our choice of standard Hermann–

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Mauguin symbols for frieze, rod and layer groups reflects the relationship between reducible space groups and subperiodic groups as their factor groups, see Section 1.2.17. In the case of the layer groups, our choice thus substantially differs from that made by Wood (1964). The interpretation of subperiodic groups as factor groups of reducible space groups also has consequences in the representation theory of space and subperiodic groups. Last but not least, this relationship reveals relations between the algebraic structure of the space group of a crystal and the symmetries of planar sections or of straight lines penetrating the crystal. These relations, analogous to the relations between the point group and symmetries of Wyckoff positions, will be described elsewhere.

It should be noted finally that all the information about scanning can be and is presented in a structure-independent way in terms of the groups involved. The scanning tables therefore extend the standard description of space groups.

5.2.2. The basic concepts of the scanning

If a crystal with a symmetry of the space group $\mathcal{G}$ is transected by a crystallographic[1] plane, called a *section plane*, then the subgroup of all elements of the space group $\mathcal{G}$ which leave the plane invariant is a layer group, which is called a *sectional layer group*, of this section plane under the action of the group $\mathcal{G}$. Analogously, if the crystal is penetrated by a crystallographic[1] straight line, called the *penetration straight line*, then the subgroup of all elements of the space group $\mathcal{G}$ which leave the straight line invariant is a rod group, which is called the *penetration rod group*, of this penetration straight line under the action of the group $\mathcal{G}$.

Sectional layer groups are therefore symmetries of crystallographic section planes and penetration rod groups are symmetries of crystallographic penetration straight lines under the action of space groups. In this sense they are analogous to site symmetries of Wyckoff positions. In addition, analogous to points, the section planes and penetration straight lines form orbits under the action of the space group $\mathcal{G}$. Planes or straight lines belonging to the same orbit have, with reference to their respective coordinate systems, the same sectional layer symmetry or penetration rod symmetry and the crystal is described in the same way with reference to any of these coordinate systems.

While every sectional layer group is, by definition, a subgroup of the corresponding space group, not every subgroup of the space group which is a layer group is necessarily a sectional layer group. Analogously, a penetration rod group is a subgroup of the corresponding space group but not every rod subgroup of a space group is a penetration rod group. It can be shown that every sectional layer group is either a maximal layer subgroup of the space group or a halving subgroup of a maximal layer subgroup, see Section 5.2.2.6.

We shall consider explicitly only the sectional layer groups, although the penetration rod groups can also be deduced from the scanning tables, see the example in Section 5.2.2.2.

5.2.2.1. The scanning for sectional layer groups

A plane in a three-dimensional space is associated with a two-dimensional vector space $V(\mathbf{a}', \mathbf{b}')$ which is called the *orientation* of the plane. If the plane of this orientation also contains a point $P + \mathbf{r}$, we shall denote it by a symbol $(P + \mathbf{r}, V(\mathbf{a}', \mathbf{b}'))$. A straight line is associated with a one-dimensional vector space $V(\mathbf{d})$ which is called the *direction* of the straight line. If the straight line of this direction also contains a point $P + \mathbf{r}$, we shall denote it by a symbol $(P + \mathbf{r}, V(\mathbf{d}))$. We assume in what follows that the vector $\mathbf{d}$ is not a linear combination of vectors $\mathbf{a}'$, $\mathbf{b}'$.

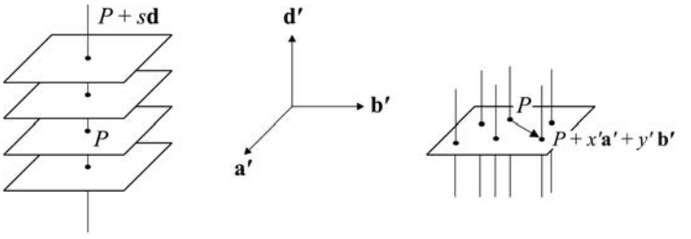

Fig. 5.2.2.1. Sets of parallel planes (left) and sets of parallel straight lines (right).

Then the set of all parallel planes with a common orientation $V(\mathbf{a}', \mathbf{b}')$ contains planes $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$. Points $P + s\mathbf{d}$ along a straight line $(P; V(\mathbf{d}))$ specify the location of individual planes as the points in which the planes intersect with the straight line $(P; V(\mathbf{d}))$ (Fig. 5.2.2.1 left). On the other hand, the set of all straight lines with a common direction $V(\mathbf{d})$ contains straight lines $(P + x'\mathbf{a}' + y'\mathbf{b}'; V(\mathbf{d}))$. The location of individual straight lines of the set is defined by their intersection points $P + x'\mathbf{a}' + y'\mathbf{b}'$ with the plane $(P; V(\mathbf{a}', \mathbf{b}'))$ (Fig. 5.2.2.1 right).

We consider now a space group $\mathcal{G}$, with a point group G and translation subgroup T_G, described by a symmetry diagram or by symmetry operations with reference to a crystallographic coordinate system $(P; \mathbf{a}, \mathbf{b}, \mathbf{c})$ (as listed, for example, in *IT* A). We want to solve the following two problems:

(1) Find the sectional layer groups $\mathcal{L}(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ which contain all those elements of $\mathcal{G}$ which leave the planes $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ invariant.

(2) Find the orbit of planes, generated by the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ under the action of the space group $\mathcal{G}$.

The general goal is to describe all possible cases, classify and systemize them. Since the first part of the problem may be described as a search for the change of the sectional layer symmetry as a plane of a given orientation changes its position so that one of its points moves along a straight line $(P; V(\mathbf{d}))$, we shall call this procedure *the scanning of the space group $\mathcal{G}$ for sectional layer groups of planes with the orientation $V(\mathbf{a}', \mathbf{b}')$ along the scanning line* $(P; V(\mathbf{d}))$. We shall use also abbreviated expressions in different contexts; for example *the scanning of the space group $\mathcal{G}$ (for layer groups)* will mean the determination of the sectional layer groups for the space group $\mathcal{G}$ and all possible orientations.

An analogous procedure is *the scanning of the space group $\mathcal{G}$ for penetration rod groups $\mathcal{R}(P + x'\mathbf{a}' + y'\mathbf{b}'; V(\mathbf{d}))$ of straight lines with the direction $V(\mathbf{d})$ along the scanning plane* $(P; V(\mathbf{a}', \mathbf{b}'))$.

Crystallographic orientations of planes are characterized by Miller (or Bravais–Miller) indices (*hkl*) [or (*hkil*)]. These indices determine a two-dimensional vector space, the orientation, all vectors of which leave the section planes with given Miller indices invariant. Those vectors of the translation group T_G (the lattice of $\mathcal{G}$) which lie in this space constitute a two-dimensional translation subgroup $T_{G1} = T(\mathbf{a}', \mathbf{b}')$ with a certain basis $(\mathbf{a}', \mathbf{b}')$. This is the group of all those translations from T_G that leave the section planes with given Miller indices invariant. This group is therefore a common translation subgroup of all sectional layer groups of section planes with these Miller indices. The vectors $\mathbf{a}'$, $\mathbf{b}'$ can be

[1] If the section plane is not crystallographic, its symmetry is not a layer group but either a rod group or a site-symmetry group. If the penetration straight line is not crystallographic, its symmetry is a site-symmetry group.

taken as the basis vectors of the two-dimensional vector space $V(\mathbf{a}', \mathbf{b}')$ and hence $T(\mathbf{a}', \mathbf{b}') = T_G \cap V(\mathbf{a}', \mathbf{b}')$.

The *scanning line* $(P; V(\mathbf{d}))$ and the *scanning direction* $V(\mathbf{d})$ are defined by a vector $\mathbf{d}$. This vector can be, quite generally, chosen as any vector complementary to the orientation $V(\mathbf{a}', \mathbf{b}')$, *i.e.* as an arbitrary vector, noncollinear with $\mathbf{a}'$, $\mathbf{b}'$, which needs not even define a crystallographic direction. Since, for a given space group $\mathcal{G}$ and orientation $V(\mathbf{a}', \mathbf{b}')$, the sectional layer group $\mathcal{L}(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ depends only on the distance of the plane from the origin P, it might seem to be of advantage to choose the direction $\mathbf{d}$ always perpendicular to $V(\mathbf{a}', \mathbf{b}')$, as in the example below. This, however, is not always the most suitable choice. We shall subordinate the choice of vector $\mathbf{d}$ to a strict convention, see Section 5.2.2.3, and call it the *scanning vector*.

Example

Consider a crystal whose space-group symmetry is *Pbcm*, D_{2h}^{11} (No. 57). The sectional layer symmetries of planes with an (001) orientation depend on the location of the plane along the line $P + z\mathbf{c}$, where the basis vector $\mathbf{c}$ is chosen as the *scanning vector* $\mathbf{d}$. If $z = 0, \frac{1}{2}$, the sectional layer group is $p2/b11$ (L16), if $z = \frac{1}{4}, \frac{3}{4}$, the sectional layer group is $pb2_1m$ (L29). The same holds if we add an integer n to the coordinate z. All these layer groups are maximal subgroups of the group *Pbcm*. The sectional layer symmetry of any other plane is a layer group $pb11$ (L12). The symbol of a layer group for a section plane located at $P + z\mathbf{c}$ is given with reference to the coordinate system $(P + z\mathbf{d}; \mathbf{a}, \mathbf{b}, \mathbf{d} = \mathbf{c})$. Notice that there are an infinite number of section planes with $z = n$ and $(n + \frac{1}{2})$ or $z = (n + \frac{1}{4})$ and $(n + \frac{3}{4})$ and an infinite number of corresponding sectional layer groups which can be written as $p2/b11$ $(n\mathbf{d})$ and $p2/b11$ $[(n + \frac{1}{2})\mathbf{d}]$ (L16) or $pb2_1m$ $[(n + \frac{1}{4})\mathbf{d}]$ and $pb2_1m$ $[(n + \frac{3}{4})\mathbf{d}]$ (L29) with reference to the coordinate system $(P; \mathbf{a}, \mathbf{b}, \mathbf{d} = \mathbf{c})$. All these groups are maximal layer subgroups of the group *Pbcm*. There are also an infinite number of section planes with other values of z which change continuously between the previously given discrete values of z; to all these section planes there corresponds one sectional layer group, $pb11$ (L12), whose Hermann–Mauguin symbol does not depend on z. This group is said to be *floating* in the direction $\mathbf{c}$ and it is a halving subgroup of all previously given sectional layer groups, see Section 5.2.2.6.

5.2.2.2. The scanning group and the scanning theorem

The main step in the solution of the scanning problem and in its tabular presentation is the introduction of the *scanning group* (Kopský, 1990), which is a central concept of scanning. This group is an intermediate product in the process for scanning of the sectional layer groups and for the penetration rod groups. We shall introduce this group with reference to the scanning for sectional layer groups. The scanning group is then a space group which depends on the *scanned* space group $\mathcal{G}$ and on the orientation $V(\mathbf{a}', \mathbf{b}')$. The prominent status of the scanning group is seen from: (i) the *scanning theorem*, which facilitates determination of the sectional layer groups as well as penetration rod groups in more complicated cases, and (ii) the convention for the choice of vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$, see Section 5.2.2.3, which standardizes the description of the scanning.

Definition of the scanning group: Let $\mathcal{G}$ be a space group with a point group G and $V(\mathbf{a}', \mathbf{b}')$ an orientation of planes, defined by Miller indices (hkl). Further let H be that subgroup of the point group G of the space group $\mathcal{G}$ that contains all those elements of G that leave the orientation $V(\mathbf{a}', \mathbf{b}')$ invariant, so that $HV(\mathbf{a}', \mathbf{b}') = V(\mathbf{a}', \mathbf{b}')$.

The space group

$$\mathcal{H} = \mathcal{H}(\mathcal{G}, (hkl)) = \mathcal{H}(\mathcal{G}, V(\mathbf{a}', \mathbf{b}')), \tag{5.2.2.1}$$

which is an *equitranslational* subgroup of the space group $\mathcal{G}$ corresponding to the point group H, is called the *scanning group* for the space group $\mathcal{G}$ and for the orientation $V(\mathbf{a}', \mathbf{b}')$ with Miller indices (hkl).

The importance of the scanning group for the scanning process is due to the following theorem (Kopský, 1990):

The scanning theorem: The scanning of the space group $\mathcal{G}$ for the sectional layer groups of section planes with an orientation $V(\mathbf{a}', \mathbf{b}')$ is identical with the scanning of the scanning group $\mathcal{H}(\mathcal{G}, (hkl)) = \mathcal{H}(\mathcal{G}, V(\mathbf{a}', \mathbf{b}'))$ for the sectional layer groups of section planes with the same orientation $V(\mathbf{a}', \mathbf{b}')$.

The scanning group $\mathcal{H}$ has, by definition, the same lattice T_G as the scanned group $\mathcal{G}$. However, the scanning group frequently belongs to a lower system than the group $\mathcal{G}$, because its point group H is a subgroup of the point group G, and its conventional basis may be different from the conventional basis of $\mathcal{G}$. In addition, the scanning group is always a *reducible* space group (Kopský, 1988, 1989*a*,*b*, 1990) because its point group H leaves the subspace $V(\mathbf{a}', \mathbf{b}')$ invariant.

Example

Consider the cubic space group $P432$ (O^1) and section planes of orientation defined by the Miller indices (001). The scanning group for this orientation is the group $P422$ (D_4^1) with reference to a basis $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$. Compare, in Part 6, Table $P432$ (O^1), the blocks headed *Linear orbit* and *Sectional layer group* $\mathcal{L}(s\mathbf{d})$ for the original scanned group and for the scanning group to see that they are identical. Moreover, we receive the same results for orientations defined by the Miller indices (100) and (010) where the scanning group is denoted by the same Hermann–Mauguin symbol $P422$ with reference to appropriate bases.

In addition, the diagram of the scanning group provides immediate information about the penetration rod groups of penetration straight lines with the direction $\mathbf{c}$ characterized by the direction indices [001]. Indeed, the spatial distribution of these rod groups is immediately seen from the diagram of the scanning group $P422$ in the basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$. For directions corresponding to the indices [100] and [010] we obtain the same results with reference to respective bases $(\mathbf{b}, \mathbf{c}, \mathbf{a})$ and $(\mathbf{c}, \mathbf{a}, \mathbf{b})$.

5.2.2.3. The conventional basis of the scanning group

In the *Scanning tables* of Part 6, we follow the usual crystallographic practice to define the orientation of planes by their Miller indices (Bravais–Miller indices in hexagonal cases). This itself already guarantees that the orientations considered are crystallographic. The choice of vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ is governed by a convention in which we distinguish the cases of orthogonal and inclined scanning.

Convention: Given the orientation of planes by Miller or Bravais–Miller indices, we choose vectors $\mathbf{a}'$, $\mathbf{b}'$ and the vector $\mathbf{d}$ of the scanning direction according to the following rules:

(i) *Orthogonal scanning*: If the scanning group $\mathcal{H}$ is of orthorhombic or higher symmetry, or if it is monoclinic with the

direction of its unique axis orthogonal to the orientation of the planes, we call the scanning *orthogonal* and the vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ are chosen in such a way that the triplet $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ constitutes a conventional right-handed basis of the scanning group $\mathcal{H}$.

(ii) *Inclined scanning*: If the scanning group is either triclinic or monoclinic with its unique axis parallel to the section planes, we call the scanning *inclined*. In this case we choose vectors $\mathbf{a}'$, $\mathbf{b}'$ in such a way that they constitute a conventional basis of the vector lattice $T(\mathbf{a}', \mathbf{b}')$, common to all sectional layer groups, while the scanning vector $\mathbf{d}$ is chosen as the shortest complementary vector.

Note that, in cases of orthogonal scanning, the first two vectors $\mathbf{a}'$, $\mathbf{b}'$ of the conventional basis of the scanning group $\mathcal{H}$ automatically constitute a conventional basis of the lattice $T(\mathbf{a}', \mathbf{b}')$ and $\mathbf{d}$ is orthogonal to the orientation $V(\mathbf{a}', \mathbf{b}')$. In cases of inclined scanning it is always possible to choose the vectors $\mathbf{a}'$, $\mathbf{b}'$ so that they constitute a conventional basis of the vector lattice $T(\mathbf{a}', \mathbf{b}')$. However, it is generally impossible to choose all three vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ as a strictly conventional basis of the scanning group because the first two vectors must lie in the space defined by Miller (Bravais–Miller) indices, which usually leads to a clash with the metric conditions as they are given, for example, in Section 9.1.4 (vi) and (vii) of *IT* A (2005).

The choice of the scanning direction $\mathbf{d}$ as that of a vector of the basis of the scanning group guarantees the periodicity $\mathbf{d}$ of the scanning. As a result, it is sufficient to describe the scanning for a given orientation, *i.e.* the sectional layer groups and orbits of planes, only in the interval with $0 \leq s < 1$ on the scanning line $P + s\mathbf{d}$. Indeed, the crystal structure of symmetry $\mathcal{G}$ is periodically repeated with periodicity $\mathbf{d}$ in the scanning direction. The sectional layer groups are, however, repeated in the scanning direction with the periodicity of the translation normalizer of $\mathcal{G}$. This is identical with the periodicity of the translation normalizer of the scanning group $\mathcal{H}$ (see the examples in Section 5.2.5.1). We recall that the translation normalizer of the space group $\mathcal{G}$, as defined by Kopský (1993*b*,*c*), is the translation subgroup of the Cheshire group (Euclidean normalizer) of $\mathcal{G}$ [see Hirschfeld (1968) and Koch & Fischer in Part 15 of *IT* A, 1987 edition or later].

In the application of the convention we note the following:

Item 1. If $G = H$ for a certain orientation of planes so that this orientation is invariant under all elements of the point group G of the space group $\mathcal{G}$, then $\mathcal{G} = \mathcal{H}$, *i.e.* the scanning group $\mathcal{H}$ coincides with the original space group $\mathcal{G}$.

The typical cases of this relationship are orientations (001) for the monoclinic, orthorhombic and tetragonal groups and the orientations (0001) for the trigonal and hexagonal groups. In these cases, the conventional basis of the original space group $\mathcal{G}$ also coincides with the conventional basis of the scanning group $\mathcal{H}$ and the group $\mathcal{H}$ is therefore represented by the same Hermann–Mauguin symbol as the group $\mathcal{G}$.

Item 2. The conventional basis of the scanning group $\mathcal{H}$ may differ from the conventional basis of the original group $\mathcal{G}$ even if these groups are identical. In this case the group is generally denoted by different Hermann–Mauguin symbols. This always happens in the cases of monoclinic and very frequently in cases of orthorhombic groups for other orientations than (001) because the conventional vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ of the scanning group $\mathcal{H}$ cannot be made identical with the conventional basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the group $\mathcal{G}$.

Example

Consider the space group $\mathcal{G} = Pmmm$ (D_{2h}^1) and the orientations described by the Miller indices (001), (100), (010). The scanning group $\mathcal{H} = \mathcal{G}$ is identical with the scanned group and its Hermann–Mauguin symbol *Pmmm* is the same for all three orientations.

If, however, the scanned group is the group $\mathcal{G} = Pmma$ (D_{2h}^5), then again the scanning group $\mathcal{H}$ is identical with the scanned group $\mathcal{G}$ for the three orientations, but the Hermann–Mauguin symbols of the scanning group are now different: they are *Pmma*, *Pmcm* and *Pbmm* for the orientations (001), (100) and (010), respectively.

Item 3. If $H \subset G$, so that the point group H is a proper subgroup of the point group G, then the conventional basis of the scanning group $\mathcal{H}$ is usually different from the conventional basis of the original group $\mathcal{G}$, although the groups are equitranslational, *i.e.* have the same translation subgroup. The conventional basis of the scanning group $\mathcal{H}$ in the case when $H \subset G$ actually coincides with the conventional basis of the space group $\mathcal{G}$ only in the cases of the orientations (001), (100) and/or (010) if $\mathcal{G}$ is cubic of lattice type P or I and hence $\mathcal{H}$ is tetragonal of the same lattice type. The centring type of the scanning group $\mathcal{H}$ is also frequently different from the centring type of the original group $\mathcal{G}$.

5.2.2.4. The types of scanning

It is useful to characterize various scanning tasks using the names of the crystallographic systems of the scanned group and of the scanning group. The scanning tables are naturally built up from lower to higher symmetries, according to the standard sequence of space groups. In this process, some already-considered space groups of lower crystallographic systems appear as scanning groups for those orientations which are not invariant under the point group G of the scanned space group $\mathcal{G}$ of a higher crystallographic system. In the first column of Table 5.2.2.1, the crystallographic systems are listed in their usual hierarchy and to the right of each system are listed the lower systems from which some groups appear as scanning groups. We use terms such as *tetragonal/monoclinic* scanning when a tetragonal space group $\mathcal{G}$ is considered and the scanning group $\mathcal{H}$ is monoclinic. Simple expressions such as *orthorhombic* scanning will mean that the scanning group $\mathcal{H}$ is orthorhombic, to distinguish it from the expression *scanning of orthorhombic groups*, which means that the original space group $\mathcal{G}$ is orthorhombic. The lattice of trigonal scanning groups in the case of *cubic/trigonal* scanning is always rhombohedral as indicated in parentheses.

Table 5.2.2.1. *Various types of scanning*

Triclinic					
Monoclinic	triclinic				
Orthorhombic	monoclinic	triclinic			
Tetragonal	orthorhombic	monoclinic	triclinic		
Trigonal	orthorhombic	monoclinic	triclinic		
Hexagonal	orthorhombic	monoclinic	triclinic		
Cubic	tetragonal	trigonal (rhombohedral)	orthorhombic	monoclinic	triclinic

5.2.2.5. Orientation orbits

The point group G of the scanned group $\mathcal{G}$ acts on the orientations defined by Miller indices (*hkl*) or Bravais–Miller indices (*hkil*). The set of all orientations $V(\mathbf{a}_i', \mathbf{b}_i')$ obtained from a given orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ by the action of the elements of the group G is called the *orientation orbit*. The point group $H_1 \subseteq G$ which leaves the orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ invariant is the point group of the scanning group $\mathcal{H}_1$ for this orientation. From the coset resolution

$$G = H_1 \cup g_2 H_1 \cup \ldots \cup g_p H_1 \qquad (5.2.2.2)$$

we obtain orientations of the orbit by the action of cosets on the first orientation: $V(\mathbf{a}_i', \mathbf{b}_i') = g_i H_1 V(\mathbf{a}_1', \mathbf{b}_1') = g_i V(\mathbf{a}_1', \mathbf{b}_1')$. In general, the number of orientations in the orbit is equal to the index $p = [G : H_1]$ of the subgroup H_1 in G. The point group $H_i \subset G$ which leaves the orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ invariant is the conjugate subgroup $H_i = g_i H_1 g_i^{-1}$ of the point group H_1 in the group G. If $H_1 = H = G$, then the scanning group $\mathcal{H}$ is identical with the scanned group $\mathcal{G}$ and the orientation orbit contains just one orientation.

In the general case, to each orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ there corresponds a scanning group $\mathcal{H}_i$, conjugate to the scanning group $\mathcal{H}_1$. The elements of a coset $g_i H_1$ send the scanning vector $\mathbf{d}_1$ for the first orientation into scanning vectors $\mathbf{d}_i = g_i H_1 \mathbf{d}_1 = g_i \mathbf{d}_1$ for orientations $V(\mathbf{a}_i', \mathbf{b}_i')$.

The set of the conjugate scanning groups $\mathcal{H}_i$ is obtained from the coset resolution of the space group, which corresponds to the coset resolution (5.2.2.2) of the point group:

$$\mathcal{G} = \mathcal{H}_1 \cup \{g_2|\mathbf{s}_2\}\mathcal{H}_1 \cup \ldots \cup \{g_p|\mathbf{s}_p\}\mathcal{H}_1. \qquad (5.2.2.3)$$

The scanning groups $\mathcal{H}_i = \{g_i|\mathbf{s}_i\}\mathcal{H}_1\{g_i^{-1}| - g_i^{-1}\mathbf{s}_i\}$ are related in the same way to the respective conventional bases $(\mathbf{a}_i', \mathbf{b}_i', \mathbf{d}_i) = (g_i\mathbf{a}_1', g_i\mathbf{b}_1', g_i\mathbf{d}_1)$ and hence they are expressed by the same Hermann–Mauguin symbols. However, the operations in the three-dimensional Euclidean space, which correspond to operations g_i on the vector space, often contain additional translations $\mathbf{s}_i$. Quite generally, the scanning for an orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ is described in the same manner with reference to the coordinate system $(P + \mathbf{s}_i; V(\mathbf{a}_i', \mathbf{b}_i', \mathbf{d}_i))$ as the scanning for the orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ is described with reference to a coordinate system $(P; V(\mathbf{a}_1', \mathbf{b}_1', \mathbf{d}_1))$.

In analogy with Wyckoff positions, see Section 8.3.2 of *IT* A, we distinguish three types of orientations and of orientation orbits:

(1) *special orientations and special orientation orbits with fixed parameters*;

(2) *special orientations and special orientation orbits with variable parameter*; and

(3) *general orientations and general orientation orbits*.

The type of the orbit is the same as the type of each of its orientations. Orientations and orientation orbits have the following characteristic properties:

(1) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *special orientation with fixed parameters* if its symmetry H is either at least orthorhombic or if it is monoclinic with the vector of its unique axis orthogonal to the orientation.

(2) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *special orientation with variable parameter* if its symmetry H is monoclinic and if it contains the vector of the unique axis.

(3) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *general orientation* if its symmetry H is triclinic.

Example 1

Orientations defined by the Miller indices (001) are special orientations with fixed parameters for monoclinic groups with unique axis c as well as for orthorhombic and tetragonal groups. Bravais–Miller indices (0001) also define special orientation with fixed parameters. In each of these cases, the orientation orbit contains just one orientation.

Orientations (010) and (100) are special orientations with fixed parameters for all orthorhombic groups and each such orientation constitutes the orientation orbit.

Orientations (001), (010) and (100) are special orientations with fixed parameters for cubic groups and they belong to the same orientation orbit.

Example 2

Orientations (*mn*0) are special orientations with variable parameter for monoclinic groups with unique axis *c*. Each such orientation constitutes an orientation orbit.

For cubic groups, the orientations (*mn*0) [with the exclusion of cases $m = \pm 1$, $n = 0$ and $m = 0$, $n = \pm 1$ in groups of Laue class $m\bar{3}$ (T_h) and also of cases $m = \pm 1$, $n = \pm 1$ in groups of Laue class $m\bar{3}m$ (O_h)] are special orientations with variable parameter. The orientation orbits contain six equivalent orientations in groups of Laue class $m\bar{3}$ (T_h) and 12 in groups of Laue class $m\bar{3}m$ (O_h), see Section 5.2.4.6.

Orientation orbits are correlated with orbits of crystal faces, see Part 10 of *IT* A. If the group H does not contain elements that change the sign of the normal, then the orientation orbit is characterized by the same set of Miller indices as the set of equivalent crystal faces. Generally, the group H contains a halving subgroup H_o whose elements leave the normal to the orientation $V(\mathbf{a}', \mathbf{b}')$ invariant while elements of the coset change its sign. In this case, the number of equivalent crystal faces is twice the number of orientations in the orbit. The group H_o is identical with the point symmetry of a crystal face of orientation $V(\mathbf{a}', \mathbf{b}')$. Such a face located at a point $P + s\mathbf{d}$ is sent to a face of the same orientation located at a point $P - s\mathbf{d}$ by those elements of H which are not contained in H_o. These are the same elements which change the direction of the scanning.

5.2.2.6. Linear orbits

We consider a section plane with orientation $V(\mathbf{a}', \mathbf{b}')$ and location $P + s\mathbf{d}$. The orbit of planes generated by the action of the scanned group $\mathcal{G}$ on this section plane splits into subsets of planes with the same orientation. The suborbit of planes with the same orientation is identical with the orbit under the action of the scanning group for this orientation. This suborbit is called the *linear orbit* of planes. If the orientation orbit contains only one orientation (scanning group = scanned group), then the linear orbit contains all planes of the orbit. If there are several orientations in the orientation orbit, then to each of these orientations there corresponds its own linear orbit. As shown in the previous section, the description of the scanning with reference to corresponding coordinate systems is identical for different orientations of the orientation orbit. The separation of planes and their sectional layer symmetries are the same in each of these orbits. In other words, the spatial distribution of layer symmetries is the same for all orientations of the orientation orbit; the scanning, however, begins generally at a point $P + \mathbf{s}_i$ for the orientation

$V(\mathbf{a}_i', \mathbf{b}_i')$. We shall concentrate our attention now to one linear orbit.

The parameter s in the description of linear orbits defines the position of the section plane by its intersection $P + s\mathbf{d}$ with the scanning line. The parameter therefore specifies the distance of the section plane from the origin P in units of $\mathbf{d}$ and is referred to as the *level* at which the section plane is located. Intersections at $P + (s + n)\mathbf{d}$, $n \in Z$ (integer) are translationally equivalent to an intersection at $P + s\mathbf{d}$ where $0 \leq s < 1$. The section planes at levels $P + (s + n)\mathbf{d}$ form an orbit under the translation group $T(\mathbf{d})$ generated by the scanning vector $\mathbf{d}$. The set of these planes is called the *translation orbit*. Each translation orbit has exactly one representative plane in the interval $0 \leq s < 1$. The linear orbit consists of one or several translation orbits.

We distinguish two types of locations and linear orbits:

(1) *Special locations of section planes and special linear orbits.*

(2) *General locations of section planes and general linear orbits.*

With reference to parameter s, the special locations always correspond to a fixed parameter, the general locations to a variable parameter. Special locations are singular in the sense that in the infinitesimal vicinity of a section plane at a special location there are only section planes of general location. The sectional layer groups corresponding to these locations have the following properties:

(1) The sectional symmetry of a plane in a special location is a layer group which contains operations changing the direction of the normal to the plane.

(2) The sectional symmetry of a plane in a general location is a layer group which does not contain operations changing the direction of the normal to the plane.

(3) The sectional symmetries of planes in special locations are always maximal layer subgroups of the space group $\mathcal{G}$ as well as of the scanning group $\mathcal{H}$. The sectional symmetry of a plane in a general location is a common halving subgroup of all sectional layer groups for special locations. We say that such a sectional layer group is *floating* in the scanning direction.

Comment: If the point group H of the scanning group $\mathcal{H}$ does not contain elements that change the normal to section planes, then all locations are general locations and there is only one sectional layer group common to all locations of section planes. The scanning group with this property is also called floating in the scanning direction.

The number of planes in a translation orbit: The total number of planes in a translation orbit is infinite because the index of the sectional layer group in the scanning group is. We can, however, count the number of planes in a translation orbit in an interval $0 \leq s < 1$. If the point group of the scanning group is H and the point group of the sectional layer group for a given translation orbit is L, then the number of planes in this orbit in the interval $0 \leq s < 1$ equals the index $[H : L]$ when the centring of the scanning group is P or C. When the centring of the scanning group is A, B, I or F, this number is $2[H : L]$; when the centring type of the scanning group is R, this number is $3[H : L]$.

The number f of planes in an orbit with a general parameter s per unit interval also defines the length of the fundamental region of the space group $\mathcal{G}$ as well as of the scanning group $\mathcal{H}$ in this interval. This length s_o is a fraction of unit interval, $s_o = \frac{1}{f}$, where $f = [H : L]$, $2[H : L]$ or $3[H : L]$ according to the centring of the scanning group and L is the point group of sectional layer groups corresponding to a general orbit.

5.2.2.7. Orthogonal, inclined and triclinic scanning

It is convenient for future reference to refine the basic categories of orthogonal and inclined scanning as follows:

(1) *Orthogonal scanning*. We call the scanning orthogonal if the scanning group is orthorhombic, tetragonal, trigonal or hexagonal.

(2*a*) *Monoclinic/orthogonal scanning*. This term is used if the scanning group is monoclinic and the vector $\mathbf{d}$ defines its unique axis.

In both cases the vector $\mathbf{d}$ is orthogonal to the vectors $\mathbf{a}'$ and $\mathbf{b}'$ and they occur whenever the orientation orbit is a special orbit with fixed parameters.

The absolute value $d = |\mathbf{d}|$ of the scanning vector is, in cases of orthogonal scanning, equal to the interplanar distance defined by the Miller indices of the orientation.

(2*b*) *Monoclinic/inclined scanning*. The scanning is called monoclinic/inclined if the scanning group is monoclinic and its unique axis is one of the vectors $\mathbf{a}'$, $\mathbf{b}'$. The vector $\mathbf{d}$ is actually not necessarily inclined to the orientation $V(\mathbf{a}', \mathbf{b}')$. It may be orthogonal owing to special metric conditions of the lattice which are determined by the scanned group $\mathcal{G}$. It is, however, a vector of a monoclinic basis which lies in the plane orthogonal to the unique axis. This case occurs when the orientation orbit is a special orbit with one variable parameter.

The interplanar distance d in the case of inclined scanning is $d = |\mathbf{d}| \cos\varphi$ where φ is the angle of the vector $\mathbf{d}$ with the normal to the plane.

(3) *Triclinic scanning*. The scanning is called triclinic or trivial if the scanning group is triclinic. This case occurs when the orientation orbit is a general orbit.

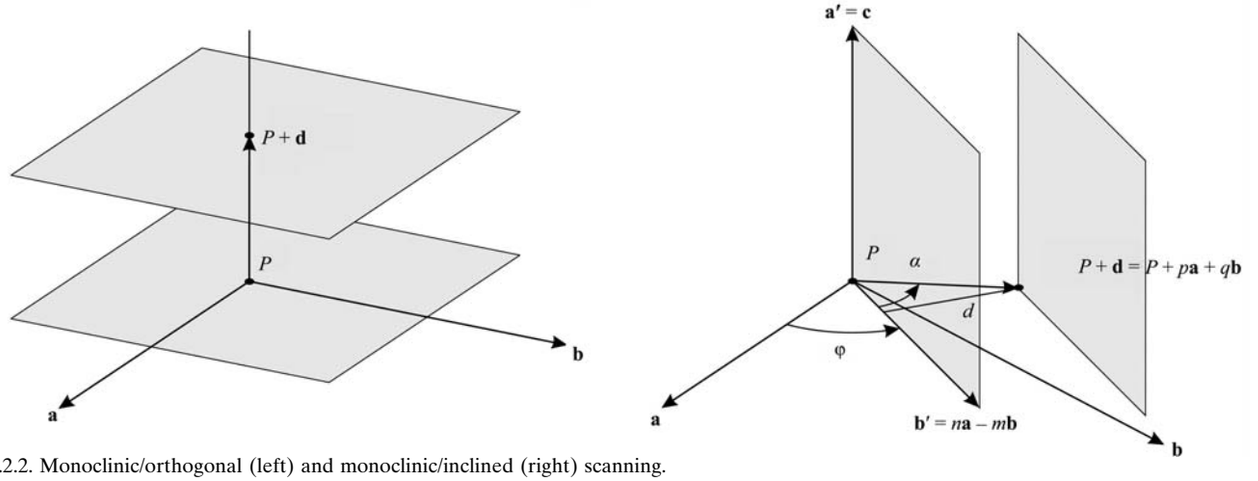

Fig. 5.2.2.2. Monoclinic/orthogonal (left) and monoclinic/inclined (right) scanning.

The difference between monoclinic/orthogonal and monoclinic/inclined scanning is illustrated in Fig. 5.2.2.2. The orientation in the first case is fixed, while the second case applies to various orientations containing the monoclinic unique axis. The orientation can be defined by one free parameter, the angle φ; we use instead Miller indices ($mn0$).

5.2.3. The contents and arrangement of the scanning tables

In the scanning tables two formats are used:

Standard format: This is the format in which the complete tables for triclinic and monoclinic groups and the tables of orthogonal scanning for all other groups are presented.

Auxiliary tables: These tables represent, in an abbreviated form, the cases where the scanned group is orthorhombic or belongs to a higher system and the orientation defines monoclinic/inclined scanning. The scanning is represented implicitly by referring to respective tables of monoclinic groups. [Note that in the online version of this volume the auxiliary tables are supplemented by explicit scanning tables.]

The tables are grouped according to crystallographic systems. Within each system, the standard-format tables are grouped into geometric classes in the same order as in *IT* A. The auxiliary tables follow the tables of standard format at the end of each Laue class.

5.2.3.1. The standard format

The content and arrangement of the standard-format tables are as follows:

(1) Headline.
(2) Orientation orbit.
(3) Conventional basis of the scanning group.
(4) Scanning group.
(5) Translation orbit.
(6) Sectional layer group.

The standard tables for triclinic groups describe the trivial scanning where the scanning group is $P1$ or $P\bar{1}$. The tables for monoclinic groups describe monoclinic/orthogonal scanning and monoclinic/inclined scanning. The standard tables for the remaining groups describe only orthogonal scanning for these groups.

5.2.3.1.1. Headline

The headline begins with the serial number of the space-group type identical with the numbering given in *IT* A, followed by a short Hermann–Mauguin symbol. The Schönflies symbol is given in the upper right-hand corner.

The next line is centred and contains the full Hermann–Mauguin symbol of the specific space group for which the scanning is described in the table. This is followed by a statement of origin in those cases where two space groups of different origin are considered, or by a statement of cell choice when different cell choices are used for a monoclinic space group.

The specific space group considered in the table is that space group, including its orientation (setting) and location (origin choice), the diagram of which is presented in *IT* A, assuming that the upper left-hand corner of the diagram represents the origin P, its left edge downwards the vector **a**, its upper edge to the right the vector **b**, while vector **c** is directed upwards. In the case of orthorhombic and monoclinic groups, this is the diagram in the (abc) setting, the so-called standard setting. For some group types, two different origins are given in *IT* A. Both are used to consider two specific groups of the same type with different locations in the present tables. The scanning for each of these groups is described in a separate table. In the case of monoclinic groups, one, three or six different cell choices, depending on the group type, are considered, see Section 5.2.4.2.

5.2.3.1.2. Orientation orbit

Each table is divided into five columns. The first column is entitled *Orientation orbit* (hkl) or *Orientation orbit* ($hkil$). The orientations are specified by their Miller or Bravais–Miller indices. Each orientation defines a row for which the scanning is described in the next columns. Orientations which belong to the same orbit are grouped together and orientation orbits are separated by horizontal double lines across the table for space groups of the tetragonal and higher-symmetry systems and for the monoclinic groups. The vertical separation for orthorhombic groups is explained in Section 5.2.4.3.

Orientation orbits are listed in each table in the following order from top to bottom:

(1) Special orientation orbits with fixed parameters which contain just one orientation. Such orbits do not occur in triclinic and cubic groups.

(2) Special orientation orbits with fixed parameters which contain several orientations. Such orbits do not occur in triclinic, monoclinic and orthorhombic groups.

(3) Special orientation orbits with variable parameter. Such orbits do not occur in triclinic groups. They are presented in standard format for monoclinic groups. In this case, the orientations are defined by Miller indices ($n0m$) (unique axis b) or ($mn0$) (unique axis c) and the orbit contains just one orientation. For higher symmetries, these orbits contain several orientations which are given in the auxiliary tables.

General orientation orbits are not included; the corresponding scanning is trivial and the presentation of these orbits would take up too much space.

5.2.3.1.3. The scanning group and its conventional basis

The second column is entitled *Conventional basis of the scanning group* and it contains three subcolumns headed by the symbols of vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$. Next to it is the third column with the heading *Scanning group* $\mathcal{H}$. In the subcolumns, the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ of the conventional bases of the scanning groups $\mathcal{H}$ are specified in terms of the conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$. The scanning groups are described in the third column by their short Hermann–Mauguin symbols.

(1) *Orbits with one orientation*: With the exception of cubic groups, all space groups are reducible so that the orientations (001) or (0001) are invariant under the point group G and the orbit contains only one orientation. The scanning group $\mathcal{H}$ in these cases is identical with the scanned group $\mathcal{G}$ and its conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) is identical with the conventional basis (**a**, **b**, **c**) so that the groups $\mathcal{G}$ and $\mathcal{H}$ are denoted by the same Hermann–Mauguin symbol. The row for this orientation is always listed first.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for the orientations (100) and (010) in orthorhombic groups. However, the Hermann–Mauguin symbol for the scanning group may differ from that of the scanned group. This is a result of having the $\mathbf{a}'$ and $\mathbf{b}'$ basis vectors of the scanning group always representing the basis vectors of the resulting sectional layer

groups. The alternative setting symbols used are those listed in Table 4.3.2.1 of Part 4 of *IT* A.

Example

Space group *Pbcn*, D_{2h}^{14} (No. 60). The group itself is the scanning group for all three orientations (001), (100) and (010). However, in view of the conventional choice of the basis of the scanning group, its symbols are *Pbcn*, *Pbna* and *Pnca*, respectively.

Monoclinic groups. The scanning group $\mathcal{H}$ coincides with the scanned group $\mathcal{G}$ for the orientations (010) (unique axis *b*) and (001) (unique axis *c*). These are the cases of monoclinic/orthogonal scanning and, according to convention, the scanning vector **d** is chosen as the vector of the unique axis. The symbol of the scanning group coincides with the Hermann–Mauguin symbol for unique axis *c* in both cases.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for orientations (*n*0*m*) (unique axis *b*) or (*mn*0) (unique axis *c*). These cases lead to monoclinic/inclined scanning described below in conjunction with the auxiliary tables. Vector $\mathbf{a}'$ is, in these cases, chosen as the vector of the unique axis. Since this vector is considered as the first vector in the conventional basis of the scanning group, the Hermann–Mauguin symbols for the scanning group are the symbols that correspond to unique axis *a*. They may differ further depending on the choice of vectors $\mathbf{b}'$ and **d**.

(2) *Orbits with several orientations*: There are several Miller indices in each box of the first column which denote the orientations belonging to one orientation orbit. In the three subcolumns of the second column, the conventional bases of the scanning groups $\mathcal{H}_i$, *i.e.* the vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$, $\mathbf{d}_i$, are specified in terms of the conventional basis vectors **a**, **b**, **c** of the space group $\mathcal{G}$ and of the Miller indices. The vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$, $\mathbf{d}_i$ then represent the conventional bases with respect to which the scanning groups $\mathcal{H}_i$ are given by their Hermann–Mauguin symbols in the third column. These scanning groups are of the same type for all orientations of the orbit and they are also oriented in the same way with respect to their bases; they may, however, have different origins. Therefore, the Hermann–Mauguin symbols of the scanning groups are the same for all orientations of a given orbit up to a possible shift of origin.

Example

Space groups $P42_12$, D_4^2 (No. 90), $P4_122$, D_4^3 (No. 91) and $P4_12_12$, D_4^4 (No. 92), the orientation orbit (100) and (010): In the case of the group $P42_12$, the scanning groups for the orientations (100) and (010) are denoted by the same symbol $P2_122_1$ with reference to coordinate systems $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; \mathbf{b}, \mathbf{c}, \mathbf{a})$ and $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$, respectively.

In the case of the group $P4_122$, the scanning group for the orientation (100) is written as $P22_12$ ($\mathbf{b}'/4$). This is equivalent to the statement that the scanning group is the group $P22_12$ with reference to coordinate system $(P + \mathbf{b}'/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$. The scanning group for the orientation (010) is the group $P22_12$ with reference to coordinate system $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

In the case of the group $P4_12_12$, we conclude analogously that the scanning group for the orientation (100) is the group $P2_12_12_1$ with reference to coordinate system $(P + 3\mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + 3\mathbf{c}/8 + \mathbf{a}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$, while for the orientation (010) it is the group $P2_12_12_1$ with reference to coordinate system $(P + \mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/8 + \mathbf{b}/4; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

The vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$ also define the translation subgroup T_{Gi} of all sectional layer groups corresponding to a given orientation, which are listed in the fifth column. The vectors either themselves constitute the conventional basis of these layer groups or the conventional basis is expressed through them.

The scanning groups $\mathcal{H}_i$ are conjugate subgroups of the space group $\mathcal{G}$ in cases when there is more than one orientation in the orbit. They are accordingly expressed by the same Hermann–Mauguin symbol with respect to different coordinate systems. There are cases when the origins of these coordinate systems for the conjugate scanning groups $\mathcal{H}_i$ coincide. In this case, one block of the table is sufficient to describe the scanning groups, the translation orbits and the corresponding sectional layer groups in the same manner as in the case of an orbit with one orientation. The common origin $P + \boldsymbol{\tau}$ is stated in a line above the block in the form 'With respect to origin at $P + \boldsymbol{\tau}$' if it is different from the origin *P* of the coordinate system of the scanned group $\mathcal{G}$.

When origins are different, there appear several blocks with Hermann–Mauguin symbols of the scanning group at different locations for different orientations. The blocks are then separated by horizontal lines through the last three columns. Two ways are used to express the fact that the origin of the scanning group does not coincide with the origin of the original group $\mathcal{G}$. We use the Hermann–Mauguin symbol of the scanning group with the statement of the shift of its origin (as a rule below the symbol) for each of the separated blocks. In some cases, for typographical reasons, we state with respect to which origin the Hermann–Mauguin symbol of the scanning group, and consequently the description of the translation orbit and of the sectional layer groups, is referring to.

5.2.3.1.4. The linear orbits and sectional layer groups

The fourth column, headed *Linear orbit* $s\mathbf{d}$, describes the linear orbits of planes for the orientation of this row and the fifth column, headed *Sectional layer group* $\mathcal{L}(s\mathbf{d})$, describes the corresponding sectional layer groups.

The location of the plane along the line $P + s\mathbf{d}$ determines a certain layer group; the symbol $\mathcal{L}(s\mathbf{d})$ next to $s\mathbf{d}$ is a shorthand for the sectional layer group $\mathcal{L}(P + s\mathbf{d}, (hkl))$ of the section plane passing through the point $P + s\mathbf{d}$ on the scanning line. $\mathcal{L}(s\mathbf{d})$, as a function of *s*, has a periodicity of the translation normalizer of the space group $\mathcal{G}$ in the direction **d** but we list the translation orbits within $0 \leq s < 1$, *i.e.* with periodicity **d**. This is important because the planes at levels separated by the periodicity of the normalizer do not necessarily belong to the same orbit.

The planes form orbits with fixed parameter *s* and with a variable parameter *s*. The orbits with fixed parameter *s* are recorded in terms of fractions of vector **d**; one of these fractions always lies in the interval $0 \leq s < s_o$, where s_o is the length of the fundamental region of the scanned group $\mathcal{G}$ along the scanning line $P + s\mathbf{d}$ in units of **d**. The fixed values of *s* are always given in the range $0 \leq s < 1$. If planes at different levels belong to the same orbit, then the levels are enclosed in square brackets. The sectional layer group corresponding to a certain level *s* is then given in the fifth column by its Hermann–Mauguin symbol in the coordinate system $(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$. If the levels on the same line refer to the same Hermann–Mauguin symbol of a sectional layer group but are not enclosed in brackets, then they belong to different orbits. The sectional layer groups belonging to different planes of the orbit are certainly of the same type and parameters but they may be oriented or located in different ways so that their Hermann–Mauguin symbols are different because they refer to the same basis $(\mathbf{a}', \mathbf{b}')$. In this case, the levels corresponding to the

same orbit are listed in a column, beginning and ending with brackets, and to each level is given the sectional layer group.

There is always only one row (which may, however, split for typographical reasons) corresponding to orbits with a variable parameter s and the one sectional layer group which is floating along the scanning direction and which is a common subgroup of all sectional layer groups for orbits with fixed parameters. This row always contains the term $s\mathbf{d}$ where s belongs to the fundamental region $0 \le s < s_o = \frac{1}{f}$ of the group $\mathcal{G}$ along the line $P + s\mathbf{d}$. Here s_o is a fraction of 1 and the region is a fraction of the interval $0 \le s < 1$. These levels correspond to locations of planes of the translation orbit along the direction $\mathbf{d}$ within the unit interval. The levels are expressed in a compact way; as a result there appears an entry $\pm s\mathbf{d}$ in cases when the scanning group is not polar. Since s is in the interval $0 \le s < s_o$, $-s$ is negative and hence not in the interval $0 \le s_i < 1$; this level is equivalent to the level $(1 - s)\mathbf{d}$.

Following each Hermann–Mauguin symbol, we give the sequential number of the type to which the sectional layer group belongs, according to its numbering in Parts 1–4 of this volume.

Example 1

Orientation orbit (001) for the space groups $P422$, D_4^1 (No. 89), $P4_222$, D_4^5 (No. 93) and $P4_122$, D_4^3 (No. 91).

Group $P422$: The entries '$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$' in the fourth column followed by $p422$ in the fifth column indicate that there are two separate translation orbits, represented by planes passing through P and $P + \frac{1}{2}\mathbf{d}$; planes of both orbits have the same sectional layer group with reference to the respective coordinate systems.

The sectional layer symmetry at a general level is $p4$ and the translation orbit contains planes at two levels (the index of the point group 4 in the point group 422), described as $[s\mathbf{d}, -s\mathbf{d}]$. It is $s_o = \frac{1}{2}$ and both levels $\pm s\mathbf{d}$ belong to the same orbit. For positive s we can change $-s$ to $(1 - s)$ to get the level in the interval $0 \le s_i < 1$.

Group $P4_222$: The entries $[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ are now enclosed between square brackets to indicate that the planes at these levels along the line $P + s\mathbf{d}$ belong to the same orbit. The sectional layer symmetry is $p222$.

The sectional layer symmetry at a general level is $p112$, so that there must be four [422 (D_4) : 122 (C_2)] levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$ where $0 < s < s_o = \frac{1}{4}$. Again we can change $-s$ to $(1 - s)$ to get the level in the interval $0 < s_i < 1$.

Group $P4_122$: The entry '$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$' in the first subrow and the entry '$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]'$ in the second subrow indicate that the planes on corresponding levels all belong to the same translation orbit. The corresponding sectional layer groups $p121$ and $p211$ for the first and second subrow are of the same type but the orientations of their twofold axes are different. The Hermann–Mauguin symbols are therefore different because they are expressed with reference to the same basis [in this case the basis $(\mathbf{a}, \mathbf{b})$].

The sectional layer symmetry at a general level is $p1$ so that $s_o = \frac{1}{8}$ and there must be eight levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$.

Example 2

We consider the group $R\bar{3}$, C_{3i}^2 (No. 148) and the orientation (0001). There are three subrows in the columns for the translation orbits and the sectional layer groups. In the first row there are the entries $[0\mathbf{d}, [\frac{1}{2}\mathbf{d}$; and $p\bar{3}$; in the second row $\frac{1}{3}\mathbf{d}$, $\| \frac{5}{6}\mathbf{d}$, and $p\bar{3}$ $[(2\mathbf{a} + \mathbf{b})/3]$; and in the third row $\frac{2}{3}\mathbf{d}]$ $\frac{1}{6}\mathbf{d}]$ and $p\bar{3}$ $[(\mathbf{a} + 2\mathbf{b})/3]$. This is to be interpreted as follows: the levels $[0\mathbf{d}, \frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}]$ belong to one translation orbit, distinct from the orbit to which belong the levels $[\frac{1}{2}\mathbf{d}, \frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}]$. The sectional layer groups are groups $p\bar{3}$ on all these levels but they are located at different distances from points $P + s\mathbf{d}$ for different levels $s\mathbf{d}$.

The sectional layer symmetry at a general level is $p3$. The point group 3 is of index 2 in the point group $\bar{3}$ and the lattice is of the type R so there are six planes in the translation orbit per unit interval along $\mathbf{d}$ and $s_o = \frac{1}{6}$. The translation orbit is described by $[\pm s\mathbf{d}, (\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{2}{3})\mathbf{d}]$.

Example 3

Space group $P4/mmm$, D_{4h}^1 (No. 123). The scanning groups for the orientations (100) and (010) which belong to the same orientation orbit are expressed by the same Hermann–Mauguin symbol $Pmmm$ in their respective bases. The translation orbits and sectional layer groups are therefore expressed in the same block.

The scanning groups for the orientations (110) and $(1\bar{1}0)$ of the same orientation orbit under the space group $P4/nbm$, D_{4h}^3 (No. 125) are expressed by the same Hermann–Mauguin symbol $Bmcm$ ($\mathbf{d}$/4) in the respective bases if the scanned group is chosen according to origin choice 1 in *IT* A. Hence the translation orbits and sectional layer groups are expressed in one block; they are the same with reference to their corresponding bases. For origin choice 2, the locations of the scanning groups are different; we obtain the group $Bmcm$ for the orientation (110) and $Bmcm$ $[(\mathbf{a}' + \mathbf{d})/4]$ for the orientation $(1\bar{1}0)$. Each of these scanning groups has its own box with the translation orbits and sectional layer groups. If we compare the two boxes, we observe that the data in the second box are the same as in the first box but shifted by $[(\mathbf{a}' + \mathbf{d})/4]$.

Example 4

Consider the block of the orientation orbit (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$ for space groups $P4_332$, O^6 (No. 212), $P4_132$, O^7 (No. 213) and $I4_132$, O^8 (No. 214). The Hermann–Mauguin symbol of the scanning group with reference to their bases is the same, $R32$, up to a shift of the origin. In the row for each orientation, therefore not only are the bases given, but also the location of the origin so that a complete coordinate system is specified in such a way that the symbol is exactly the same for each orientation. The symbol of the scanning group, the location of the orbits and the sectional layer groups are given in the last block; all this information is formally the same but for each orientation it refers to its own coordinate system.

5.2.3.2. Auxiliary tables

The auxiliary tables describe cases of monoclinic/inclined scanning for groups of orthorhombic and higher symmetries. They are clustered together for groups of each Laue class, starting from Laue class D_{2h} – mmm, after the tables of orthogonal scanning, *i.e.* after the standard-format tables for this Laue class.

All possible cases of monoclinic/inclined scanning reduce to cases where the scanned group $\mathcal{G}$ itself is monoclinic and the orientation is defined by the Miller indices ($mn0$). These cases are described as a part of the standard-format tables for monoclinic groups. Two bases are used in this description:

(i) The conventional basis (**a**, **b**, **c**) of the group $\mathcal{G}$ in its role as the scanned group.

(ii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) (**a**′, **b**′, **d**) of the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group.

If the scanned group $\mathcal{G}$ is of higher than monoclinic symmetry, then the monoclinic scanning group $\mathcal{H} \subset \mathcal{G}$ and we use three bases:

(i) The conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$.

(ii) The conventional basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of the monoclinic scanning group $\mathcal{H}$, which is further called the *auxiliary basis*. This basis is always chosen so that the vector $\widehat{\mathbf{c}}$ is the unique axis vector.

(iii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) (**a**′, **b**′, **d**) of the scanning group $\mathcal{H}$.

Two types of tables from which orbits of planes and sectional layer groups can be deduced are given:

(1) *Tables of orientation orbits and auxiliary bases of scanning groups*. These contain Miller indices of orientations in the orbit and define auxiliary bases ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of the respective scanning groups in terms of the basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$ and of the Miller indices of the orientation.

(2) *Reference tables*. These serve to give a reference to that table of a monoclinic group from which one can read the scanning data.

In the next two sections we describe the construction of these two types of tables and their use in detail.

5.2.3.2.1. Tables of orientation orbits and auxiliary bases of scanning groups

The cases of monoclinic/inclined scanning occur when the orientation of the section plane:

(i) contains the direction of some symmetry axis of even order [scanning group of geometric class 2 (C_2)],

(ii) is orthogonal to a symmetry plane [scanning group of geometric class m (C_s)],

(iii) contains the direction of some symmetry axis of even order and at the same time is orthogonal to a symmetry plane [scanning group of geometric class $2/m$ (C_{2h})].

Auxiliary basis of the scanning group. In each of these cases, there is a set of orientations for which the property (i), (ii) or (iii) is common and all orientations of this set contain the vector that defines the unique axis of a monoclinic scanning group which is also common for all orientations of the set. An auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of this scanning group is defined with reference to that one orientation of the set which is described by Miller indices (mn0).

The first column of each table describes orientations of the orbit by Miller indices with reference to the conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$. Various possible situations can be distinguished by three criteria:

(1) The structure of orbits.

(i) All orientations of the orbit contain the vector of the unique axis of the scanning group. This also means that there is only one scanning group for all orientations of the orbit.

This situation occurs for orientations that contain the vector of principal axis c in tetragonal and hexagonal groups. It occurs also for orientations which contain the vector of any of the orthorhombic axes c, a or b.

(ii) The orbit splits into sets of orientations where each set has its own common unique axis and scanning group.

This situation occurs for orientations that contain vectors of auxiliary axes of groups of Laue classes $4/mmm$ (D_{4h}), $\bar{3}m$ (D_{3d}), $6/mmm$ (D_{6h}), $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h).

(2) Possible increase of the symmetry for special orientations.

(i) All orientations of the set with common unique axis have the same monoclinic scanning group.

This is the case of groups of Laue classes $4/m$ (C_{4h}) and $6/m$ (C_{6h}), and of orientations that contain the vector **c** of the principal axis.

(ii) In all other cases there appear special orientations in the set which have higher symmetry than monoclinic.

(3) Auxiliary basis of the scanning group.

The auxiliary bases of scanning groups are their conventional bases corresponding to unique axis c.

(i) If the conventional basis of the scanning group can be based on the same vectors as the conventional basis of the scanned group, parameters m, n are used in the Miller indices that define the orientation.

(ii) If the conventional basis of the scanning group cannot be based on the same vectors as the conventional basis of the scanned group, parameters h, k, l are used in the Miller indices that define the orientation with reference to the conventional basis (**a**, **b**, **c**).

In these cases, the transformation of Miller indices with reference to the conventional basis (**a**, **b**, **c**) to Miller indices with reference to auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) is given in a row under the orientation orbit. The letters m and n are always used for Miller indices with reference to auxiliary bases.

The second column assigns to each orientation the conventional basis (**a**′, **b**′, **d**) of the monoclinic scanning group that is related to the auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) given in the third column in the same way as to the standard basis (**a**, **b**, **c**) in the case of monoclinic groups.

The conventional basis (**a**′, **b**′, **d**) is always chosen so that its first vector **a**′ is the vector of the common unique axis. Vector **b**′ is defined by the orientation of section planes and hence by Miller indices (either directly or indirectly through transformation to a monoclinic basis). There is the same freedom in the choice of the scanning direction **d** as in the cases of monoclinic/inclined scanning in the case of monoclinic groups.

5.2.3.2.2. Reference tables

Each table of orientation orbits for a certain centring type(s) is followed by reference tables which are organized by arithmetic classes belonging to this centring type(s). The scanned space groups $\mathcal{G}$ are given in the first row by their sequential number, Schönflies symbol and short Hermann–Mauguin symbol. They are arranged in order of their sequential numbers unless there is a clash with arithmetic classes; a preference is given to collect groups of the same arithmetic class in one table. If space allows it, groups of more than one arithmetic class are described in one table.

The first column is identical with the first column of the table of orientation orbits. On the intersection of a column which specifies the scanned group $\mathcal{G}$ and of a row which specifies the orientation by its Miller (Bravais–Miller) indices is found the scanning group, given by its Hermann–Mauguin symbol with reference to the auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$). This symbol, which may also contain a shift of origin, instructs us which monoclinic scanning table to consult. The vectors **a**′, **b**′, **d** that determine the lattice of sectional layer groups and the scanning direction are those given in the table of orientation orbits. Depending on the values of para-

meters m, n, p, q we find the scanning group in its basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) and the respective sectional layer groups.

5.2.4. Guidelines for individual systems

5.2.4.1. Triclinic system

The triclinic groups are trivial even from the viewpoint of scanning but it is nontrivial to express the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ in terms of vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and of Miller indices (hkl). Since the groups are related in the same way with respect to any given basis, we do not identify bases in the two tables. The specification *Any admissible choice* for the scanning group means that the vectors $\mathbf{a}'$, $\mathbf{b}'$ have to be chosen as a basis of the translation group in the subspace defined by Miller indices and $\mathbf{d}$ should be the vector that completes the basis of the translation group in the whole space.

The scanned groups are identical with the scanning group for all orientations in the triclinic groups $P1$, C_1^1 (No. 1) and $P\bar{1}$, C_i^1 (No. 2). There is only one orientation in each orientation orbit. In the case of the group $P1$, C_1^1 (No. 1), there is one type of linear orbit consisting of planes generated by translations $\mathbf{d}$ from either one of the set and the respective layer symmetries are the trivial groups $p1$ (L01). In the case of the group $P\bar{1}$, C_i^1 (No. 2), the orbit with a general location consists of a pair of planes, located symmetrically from a symmetry centre at distances $\pm s$ in the scanning direction $\mathbf{d}$, which is then periodically repeated with periodicity $\mathbf{d}$; the sectional layer symmetry of these planes is $p1$ (L01). Furthermore, there are two linear orbits corresponding to positions $0\mathbf{d}$ and $\frac{1}{2}\mathbf{d}$, each of which consists of a periodic set of planes with periodicity $\mathbf{d}$; the sectional symmetry in each of these cases is $p\bar{1}$ (L02).

The triclinic scanning also applies to general orientation orbits of all space groups of higher symmetry than triclinic. If the space group $\mathcal{G}$ is noncentrosymmetric, then the number of orientations in the orientation orbit is the order $|G|$ of the point group G and the linear orbits are described for each orientation as in the case of the group $P1$, C_1^1 (No. 1). If the space group $\mathcal{G}$ is centrosymmetric, then the number of orientations in the orientation orbit is $|G|/2$ and the linear orbits are described for each orientation as in the case of the group $P\bar{1}$, C_i^1 (No. 2).

5.2.4.2. Monoclinic system

The scanning of monoclinic groups is nontrivial if the section planes are either orthogonal to or parallel with the unique axis. The first case results in monoclinic/orthogonal scanning, the second in monoclinic/inclined scanning.

Depending on the space-group type, a monoclinic group $\mathcal{G}$ admits one, three or six cell choices, which are illustrated and labelled by numbers 1, 2, 3 and $\widetilde{1}$, $\widetilde{2}$, $\widetilde{3}$ in Fig. 5.2.4.1. For each cell choice, a separate table is given in which the group is specified by Hermann–Mauguin symbols with reference to unique axis b or to unique axis c.

Monoclinic/orthogonal scanning. There exists only one orientation orbit and it contains just one orientation. When the c axis is chosen as the unique axis, the scanning group $\mathcal{H}$ is not only identical with the monoclinic space group $\mathcal{G}$ considered but it also has the same Hermann–Mauguin symbol. The vectors $\mathbf{a} = \mathbf{a}'$ and $\mathbf{b} = \mathbf{b}'$ of the monoclinic basis are taken as basis vectors of the lattices of sectional layer groups and the vector $\mathbf{c} = \mathbf{d}$ defines the scanning direction.

The Hermann–Mauguin symbol of the scanned group $\mathcal{G}$ changes with reference to a basis in which the b axis is chosen as the unique axis. However, the Hermann–Mauguin symbol of the group in its role as the scanning group does not change, because the basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$.

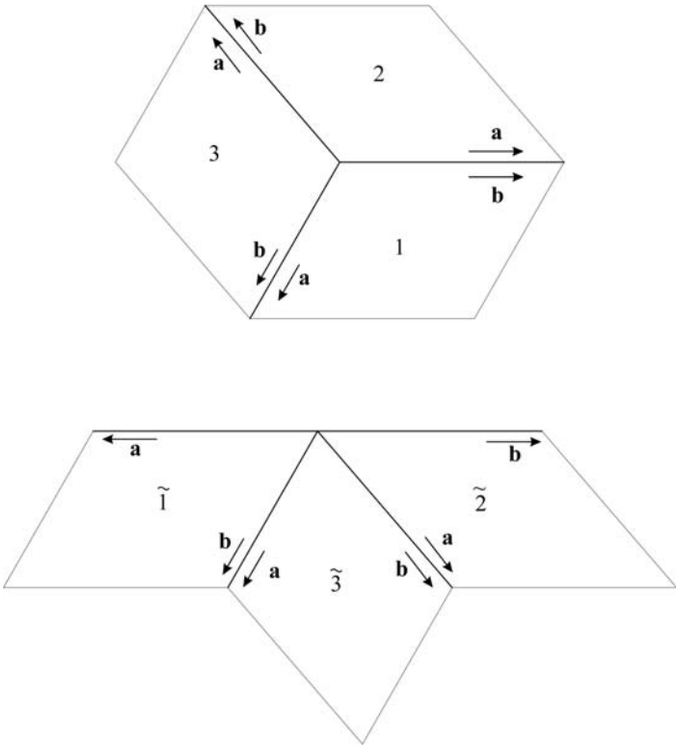

Fig. 5.2.4.1. Six monoclinic cell choices.

Monoclinic/inclined scanning. There exists an infinite number of orientations for which the section planes are parallel with the unique axis. When the c axis is chosen as the unique axis, the orientations are specified by Miller indices ($mn0$). Each orientation orbit contains again just one orientation and the scanning group $\mathcal{H}$ is identical with the space group $\mathcal{G}$. The lattice of each sectional layer group is either a primitive or centred rectangular lattice with basis vectors $\mathbf{a}' = \mathbf{c}$ and $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$. The scanning direction is generally inclined to this orientation and the vector $\mathbf{d}$ can be chosen as any vector of the form $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$, where p, q are integers that satisfy the condition $nq + mp = 1$ so that the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ constitute a conventional unit cell of the scanning group, see Section 5.2.2.3.

The Hermann–Mauguin symbols for the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group are different to the symbol that specifies it as the scanned group because they refer to the choice of basis where the unique axis is defined by the vector $\mathbf{a}'$. The choice of the pair of vectors $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$ and $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$ defines a cell choice to which the Hermann–Mauguin symbol of the group $\mathcal{H} = \mathcal{G}$ as the scanning group refers. Notice that the vector $\mathbf{b}'$ is defined by Miller indices ($mn0$) while freedom in the choice of the scanning direction $\mathbf{d}$ remains. The choice of vector $\mathbf{d}$ may influence the Hermann–Mauguin symbols of the scanning group and of the sectional layer groups but it does not change the groups.

When the b axis is chosen as the unique axis, the orientations of section planes are defined by Miller indices ($n0m$) and the conventional basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = n\mathbf{c} - m\mathbf{a}$, $\mathbf{d} = pc + q\mathbf{a}$. The symbols of the group in its role as the scanning group for various parities of integers n, m, p and q, the linear orbits and the sectional layer groups are the same as in the case of unique axis c.

The cases of monoclinic/inclined scanning appear in all groups of higher symmetries than monoclinic for those orientations for which the scanning group is monoclinic. These cases are collected in the auxiliary tables where reference to the monoclinic/inclined part of the monoclinic scanning tables is given in each particular case.

5.2.4.3. Orthorhombic system

All groups of the orthorhombic system belong to Laue class *mmm* (D_{2h}). The standard-format tables are given first for the geometric classes 222 (D_2), *mm*2 (C_{2v}) and *mmm* (D_{2h}). These are followed by the auxiliary tables.

5.2.4.3.1. Orthogonal scanning, standard tables

Orientation orbits (001), (100) and (010): These three orientation orbits represent all orbits with fixed parameters in the orthorhombic system. Each of these consists of a single orientation. Hence the scanning group $\mathcal{H}$ for each of these orientations and for any orthorhombic group $\mathcal{G}$ coincides with the group $\mathcal{G} = \mathcal{H}$ itself. The Hermann–Mauguin symbols of the scanning groups are, however, generally different for the three orientations because they refer to different bases $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}' = \mathbf{d}$. For the orientation (001) they always coincide with the Hermann–Mauguin symbol used in *IT* A.

The scanning groups for groups of geometric classes 222 (D_2) and *mmm* (D_{2h}) are not only the same (identical with the scanned group) for all three orientations, but in a few cases they also have the same Hermann–Mauguin symbols, so the entries in the columns of the scanning group and of the sectional layer groups coincide. The orbits are separated by horizontal lines in the first column and further through the column with the scanning group, orbits and sectional layer groups, if they are different; when the Hermann–Mauguin symbol of the scanning group and hence the two remaining columns are identical, we give them as a common row for all the three orbits, which are then separated only in the first two columns. In the tables for groups of geometric class *mm*2 (C_{2v}), the orbit (001) is separated by double lines across the table from the remaining orbits (100) and (010), which are separated by single lines across the tables.

The bases for the scanning groups and for the sectional layer groups associated with these orbits are chosen in a standard manner for all orthorhombic groups:

(1) For the orientation (001), it is natural to choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \mathbf{d} = \mathbf{c}$. The symbol of the scanning group then coincides with the symbol of the space group itself, *i.e.* its symbol in the (*abc*) setting.

(2) The scanning direction for orientations (100) and (010) are along $\mathbf{d} = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$, respectively. We choose the remaining vectors $\mathbf{a}'$, $\mathbf{b}'$ in such a way that ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) is a right-handed basis, hence $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$ for the orientation (100) and $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ for the orientation (010). Accordingly, the Hermann–Mauguin symbols for the scanning groups are the symbols which correspond to the settings (*bac*) and ($\bar{c}\bar{a}b$), respectively.

5.2.4.3.2. Inclined scanning, auxiliary tables

Orientation orbits (*mn*0), (0*mn*) *and* (*n*0*m*): Each of these orientations has a scanning group of monoclinic symmetry, namely: 2 (C_2) for space groups of the geometric class 222 (D_2) in all settings and for the groups of the class *mm*2 (C_{2v}) in the (*abc*) setting; *m* (C_s) for groups of the geometric class *mm*2 (C_{2v}) in the settings (*bac*), ($c\bar{a}b$); and 2/*m* (C_{2h}) for groups of the geometric class *mmm* (D_{2h}) in all settings. In each case, the scanning group $\mathcal{H}$ is a halving subgroup of the scanned group $\mathcal{G}$ and consequently each orientation orbit contains two orientations with the same scanning group. The symmetry increases to orthorhombic and the orbit contains one orientation for the special values $m = \pm 1$, $n = 0$ or $m = 0$, $n = \pm 1$.

The scanning groups are monoclinic and one can deduce them by viewing the diagrams of the scanned groups. By omitting the axes parallel with and planes perpendicular to the diagram plane, the diagram of the scanning group remains. This, however, is the diagram of the monoclinic scanning group in its standard setting when the unique axis is perpendicular to the plane of the diagram. This unique axis is a common direction for both orientations of the orbit and it is the *c* axis for the orientation orbit (*mn*0), and the *a* axis and *b* axis for the orientation orbits (0*mn*) and (*n*0*m*), respectively. The basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ for the scanning group is expressed in the same way through the auxiliary basis and the scanning groups in the reference tables are given by their Hermann–Mauguin symbols with reference to the auxiliary bases. The three orbits are separated by horizontal lines in the tables of orientation orbits as well as in the first column of the reference tables. If the scanning group in a column for a certain scanned group $\mathcal{G}$ has the same symbol for orbits in adjoining rows, we give it in a block common to these orbits.

Transformation of Miller indices for centred cases: In the table of orientation orbits for the *C* centring, we denote the orientation of the first orbit by (*hk*0) and ($\bar{h}k$0), *i.e.* we use letters *h* and *k* instead of *m* and *n*. The letters *m* and *n* are used for the Miller indices with respect to an auxiliary basis.

The scanning group is an equitranslational subgroup of the orthorhombic scanned group. Since the scanning group is monoclinic, the orthorhombic *C* lattice is considered as a monoclinic *P* lattice (with degenerate parameters) for which we choose the auxiliary basis vectors as $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = (\mathbf{a} + \mathbf{b})/2$ and the unique axis vector $\widehat{\mathbf{c}} = \mathbf{c}$.

The orientations are, however, defined by Miller indices (*hk*0) with respect to the conventional basis (**a**, **b**, **c**) of the orthorhombic group, while the numbers *m*, *n* define the Miller indices (*mn*0) with respect to the auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$). The scanning can be found at once from tables of scanning of monoclinic groups in terms of parities of *m*, *n*, and of *p*, *q*, where $\mathbf{b}' = n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$ is determined by the orientation (*hk*0) and *p*, *q* determine the scanning direction $\mathbf{d} = p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$. Substituting for $\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$ in vectors $\mathbf{b}'$ and $\mathbf{d}$, we get

$$\widehat{\mathbf{b}} = \frac{n-m}{2}\mathbf{a} - \frac{n+m}{2}\mathbf{b} = k\mathbf{a} - h\mathbf{b}, \qquad (5.2.4.1)$$

so

$$k = \frac{n-m}{2}, \quad h = \frac{n+m}{2} \qquad (5.2.4.2)$$

and conversely

$$n = h + k, \quad m = k - h. \qquad (5.2.4.3)$$

If *h* is even and *k* odd, or *h* odd and *k* even, then both *n* and *m* are odd. However, if both *h* and *k* are odd (they cannot be simultaneously even), then both *n* and *m* are even, so that they cannot play the role of Miller indices, though they give the correct direction of the vector $\mathbf{b}'$. Dividing both by two, we get the Miller indices ($\frac{n}{2}\frac{m}{2}0$) and either the case $\frac{n}{2}$ odd, $\frac{m}{2}$ even or the case $\frac{n}{2}$ even, $\frac{m}{2}$ odd may occur. Both $\frac{n}{2}$ and $\frac{m}{2}$ cannot be simultaneously either even or odd because in these cases both *h* and *k* will be even.

The same situation occurs for the orbit (0*mn*) of *A*-centred orthorhombic groups of the class *mm*2 (C_{2v}), where the vector **a** plays the role of the unique monoclinic axis, and for all three orientation orbits (*mn*0), (0*mn*) and (*n*0*m*) in the case of *F*-centred orthorhombic groups. In the latter case, the monoclinic scanning group is of the *I*-centred type with respect to the auxiliary bases while its centring in the bases (**a**′, **b**′, **d**) depends on the choice of *n*, *m* (*via h*, *k*), and of *p*, *q*, see the monoclinic cases.

Whenever a transformation of Miller indices is used, it is printed in a special row across the table below the respective orbit; the transformation is the same for all three orbits in the case of *F* centring and is given once below the orbits.

5.2.4.4. Tetragonal system

The scanning in the tetragonal system has a slightly different character for groups of Laue class 4/*m* (C_{4h}) from those of Laue class 4/*mmm* (D_{4h}).

5.2.4.4.1. Orthogonal scanning, standard tables

Orientation orbit (001): This orbit with a single special orientation appears in all tetragonal groups. In each case, the tetragonal group itself is the scanning group for this orientation. For those tetragonal groups that are presented in *IT* A with two origin choices, we specify the scanning group by its Hermann–Mauguin symbol and origin choice in parentheses (usually below the symbol). The scanning groups are expressed with respect to bases identical with the original basis, so that the Hermann–Mauguin symbol of the scanning group is identical with the Hermann–Mauguin symbol of the scanned group including the origin choice, $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ are the vectors of the conventional basis for the sectional layer groups and the scanning direction $\mathbf{d} = \mathbf{c}$ is along the main axis. In the same way, we will later refer to tetragonal scanning groups when performing the scanning of cubic groups. There are no other orientation orbits with fixed parameters for groups of classes 4 (C_4), $\bar{4}$ (S_4) and 4/*m* (C_{4h}), *i.e.* for the groups of Laue class 4/*m* (C_{4h}).

Orientation orbit (100): This orbit contains orientations (100) and (010); it appears in groups of geometric classes 422 (D_4), 4*mm* (C_{4v}), $\bar{4}2m$ or $\bar{4}m2$ (D_{2d}), and 4/*mmm* (D_{4h}), which belong to the Laue class 4/*mmm* (D_{4h}), but not in the groups of Laue class 4/*m* (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$ for the orientation (100) and as $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{b}$ for the orientation (010). The corresponding scanning groups are orthorhombic and of the same centring type as the scanned group. In the majority of cases, the scanning groups are the same (*i.e.* expressed by the same Hermann–Mauguin symbol, with or without a shift) with respect to the two coordinate systems (*P*; $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$) and (*P*; $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}, \mathbf{d} = \mathbf{b}$) where *P* is the origin of the original group. In these cases, only one Hermann–Mauguin symbol (with or without a shift) is given for both orientations and one corresponding column of linear orbits and of sectional layer groups. Whenever this is not the case, the scanning group for one of the orientations is shifted with reference to its coordinate system as compared with the location of the other scanning group with reference to its coordinate system. There is also a respective shift of orientation orbits and of corresponding sectional layer groups. In these cases, the orientation-orbit row is split into two parts, each referring to one orientation of the orbit.

Orientation orbit (110): The orbit contains the orientations (110) and (1$\bar{1}$0); it again appears in all groups of the geometric classes 422 (D_4), 4*mm* (C_{4v}), $\bar{4}2m$ (D_{2d}) and 4/*mmm* (D_{4h}) belonging to the Laue class 4/*mmm* (D_{4h}), but not in the groups of Laue class 4/*m* (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$ for the orientation (110) and as $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation (1$\bar{1}$0). The resulting scanning groups are again orthorhombic of centring type *C* (denoted by *B* in view of the choice of the basis) when the original tetragonal group is of the type *P* and of centring type *F* when the original tetragonal group is of the type *I*. The scanning group, respective linear orbits and sectional layer groups are either the same with reference to the coordinate systems (*P*; $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$) and (*P*; $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$) or one of them is shifted with respect to the other. Accordingly, the row for the orbit either does not split or it splits into two subrows for the two orientations.

5.2.4.4.2. Inclined scanning, auxiliary tables

Orientation orbits (*mn*0) occur in groups of both tetragonal Laue classes 4/*m* (C_{4h}) and 4/*mmm* (D_{4h}). Orientation orbits (0*mn*) occur only in groups of the Laue class 4/*mmm* (D_{4h}).

Orientation orbits (*mn*0): These orbits contain two orientations, namely (*mn*0) and ($\bar{n}m$0) in groups of the geometric classes 4 (C_4), $\bar{4}$ (S_4) and 4/*m* (C_{4h}) which belong to the Laue class 4/*m* (C_{4h}), and four orientations, namely (*mn*0), ($\bar{n}m$0), ($\bar{m}n$0) and (*nm*0) in groups of the geometric classes 422 (D_4), 4*mm* (C_{4v}), $\bar{4}2m$ (D_{2d}) and 4/*mmm* (D_{4h}) which belong to the Laue class 4/*mmm* (D_{4h}).

For special values $m = 1$ and $n = 0$, the orbit contains only two orientations (100) and (010) which form an orbit with fixed parameters with an orthorhombic scanning group for groups of the Laue class 4/*mmm* (D_{4h}). For groups of the Laue class 4/*m* (C_{4h}) these two orientations represent just one particular case of the orbit (*mn*0). Analogously, the orbit with two orientations (110) and (1$\bar{1}$0) for groups of the Laue class 4/*mmm* (D_{4h}) is an orbit with fixed parameters $m = 1$, $n = 1$ while for groups of the Laue class 4/*m* (C_{4h}) it is a particular case of the orbits (*mn*0).

There are no other special orbits with variable parameter in groups of the Laue class 4/*m* (C_{4h}). Auxiliary bases are defined by one table common for both centring types *P* and *I*.

Auxiliary bases for this orbit are also common for both centring types in groups of the Laue class 4/*mmm* (D_{4h}) and they are given in the tables of orientation orbits for both types.

Orientation orbits (0*mn*): These orbits, consisting of orientations (0*mn*), (0$\bar{m}n$), (*m*0*n*) and (*m*0$\bar{n}$), appear only in groups of the Laue class 4/*mmm* (D_{4h}). The first two orientations contain the vector **a**, the other two contain the vector **b**, scanning groups are monoclinic with unique axes along vectors **a** and **b**, respectively, for the first and second pair of orientations; the scanning is inclined because the vectors **a** and **b** lie in the respective orientations. To primitive and centred lattices of the scanned groups there correspond primitive and centred lattices of the scanning groups, respectively, which is reflected in the reference tables.

Auxiliary bases for this orbit are common for both centring types in groups of the Laue class 4/*mmm* (D_{4h}) and they are given in tables of orientation orbits for both types.

For special values of parameters, the orbit coincides either with the orbit (100), (010) or with the orbit (110), (1$\bar{1}$0).

Orientation orbits (*hhl*): These orbits, consisting of orientations (*hhl*), ($\overline{h}\overline{h}l$), ($h\bar{h}l$) and ($\bar{h}hl$), appear again only in groups of the Laue class 4/*mmm* (D_{4h}). The first two orientations contain the vector $(\mathbf{a} - \mathbf{b})$, the other two contain the vector $(\mathbf{a} + \mathbf{b})$, scanning groups are monoclinic with unique axes along these vectors $(\mathbf{a} - \mathbf{b})$ and $(\mathbf{a} + \mathbf{b})$, respectively, for the first and second

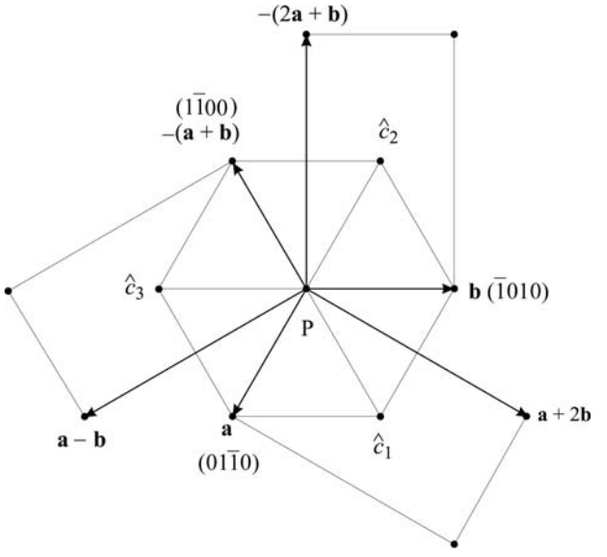

Fig. 5.2.4.2. Symbols for a hexagonal lattice with a rectangular point group.

pair of orientations; the scanning is again inclined because the vectors $(\mathbf{a}-\mathbf{b})$ and $(\mathbf{a}+\mathbf{b})$ lie in the respective orientations.

The auxiliary bases for the monoclinic scanning groups in the case of a primitive (P) tetragonal lattice are chosen as

$$\widehat{\mathbf{a}}=\mathbf{a}+\mathbf{b},\ \ \widehat{\mathbf{b}}=\mathbf{c}\ \text{ and }\ \widehat{\mathbf{c}}=\mathbf{a}-\mathbf{b} \tag{5.2.4.4}$$

for the first pair of orientations and as

$$\widehat{\mathbf{a}}=\mathbf{b}-\mathbf{a},\ \ \widehat{\mathbf{b}}=\mathbf{c}\ \text{ and }\ \widehat{\mathbf{c}}=\mathbf{a}+\mathbf{b} \tag{5.2.4.5}$$

for the second pair of orientations.

The auxiliary bases for the monoclinic scanning groups in the case of an I-centred tetragonal lattice are chosen as

$$\widehat{\mathbf{a}}=(\mathbf{a}+\mathbf{b}+\mathbf{c})/2,\ \ \widehat{\mathbf{b}}=\mathbf{c}\ \text{ and }\ \widehat{\mathbf{c}}=(\mathbf{a}-\mathbf{b}) \tag{5.2.4.6}$$

for the first pair of orientations and as

$$\widehat{\mathbf{a}}=(\mathbf{b}-\mathbf{a}+\mathbf{c})/2,\ \ \widehat{\mathbf{b}}=\mathbf{c}\ \text{ and }\ \widehat{\mathbf{c}}=(\mathbf{a}+\mathbf{b}) \tag{5.2.4.7}$$

for the second pair of orientations.

A vector parallel with planes of orientation (hhl) and orthogonal to $\mathbf{a}-\mathbf{b}$ is a multiple of

$$2h\mathbf{c}-l(\mathbf{a}+\mathbf{b}). \tag{5.2.4.8}$$

In terms of Miller indices ($mn0$) with reference to the first auxiliary basis for a P-centred lattice, such a vector is a multiple of

$$m\mathbf{c}-n(\mathbf{a}+\mathbf{b}) \tag{5.2.4.9}$$

and in terms of Miller indices ($mn0$) with reference to the first auxiliary basis for an I-centred lattice, it is a multiple of

$$(2m-n)\mathbf{c}-n(\mathbf{a}+\mathbf{b}). \tag{5.2.4.10}$$

Therefore, for a P-centred lattice, the pair of numbers (m, n) must be proportional to the pair $(2h, l)$. Since Miller indices must be relatively prime, we get $n = l$, $m = 2h$ if l is odd and $n = l/2$, $m = h$ if l is even.

For an I-centred lattice, the pair of numbers $(2m-n, n)$ must be proportional to the pair $(2h, l)$ and hence the pair $(2m, n)$ must be proportional to the pair $(2h+l, l)$. If l is odd, then $2h+l$ is also odd and we put $m = 2h+l$, so that $n = 2l$. If l is even, we put $n = l$ and $m = h+l/2$.

These relations are printed in the last rows across the tables of orientation orbits within the block for orbit (hhl).

5.2.4.5. Hexagonal family

The family splits into the trigonal and the hexagonal system. With the exception of seven group types with rhombohedral lattices [$R3$, C_3^4 (No. 146); $R\bar{3}$, C_{3i}^2 (No. 148); $R32$, D_3^7 (No. 155); $R3m$, C_{3v}^5 (No. 160); $R3c$, C_{3v}^6 (No. 161); $R\bar{3}m$, D_{3d}^5 (No. 166); and $R\bar{3}c$, D_{3d}^6 (No. 167)] all space groups of both systems have a primitive hexagonal lattice. Scanning tables are given in the hexagonal coordinate system for all groups with this lattice and the bases of the scanning groups for individual orientations are chosen identically. For the seven groups with rhombohedral lattices, the description of scanning in the hexagonal coordinate system differs from the description in the rhombohedral coordinate system only in the specification of orientations by Bravais–Miller and Miller indices, respectively. The column *Orientation orbit* is split into two columns with the headings Hexag. axes and Rhomb. axes.

5.2.4.5.1. Orthogonal scanning, standard tables

Orientation orbit (0001): The orientation (0001) is invariant under all point groups of the family; it forms therefore an orientation orbit with a single special orientation in all space groups of the family and the scanning groups for this orientation coincide with the scanned groups. We choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$ in primitive as well as in rhombohedral cases; in the latter case, the orientation is also specified in the second column as (111). The Hermann–Mauguin symbols of the scanning groups also coincide with the symbols of the scanned groups; to specify both the scanned and the scanning groups with rhombohedral lattices with reference to hexagonal bases we use an obverse setting as in *IT* A.

All corresponding sectional layer groups have the same planar hexagonal lattice with basis vectors $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The basis $(\mathbf{a}, \mathbf{b})$, denoted as usual by p, is the conventional basis for all trigonal/hexagonal, hexagonal/hexagonal, monoclinic/oblique and triclinic/oblique sectional layer groups. To describe the monoclinic/rectangular and orthorhombic/rectangular sectional layer groups, we choose three conventional rectangular bases: $\widehat{c}_1 = (\mathbf{a}, \mathbf{a}+2\mathbf{b})$, $\widehat{c}_2 = (\mathbf{b}, -(2\mathbf{a}+\mathbf{b}))$ and $\widehat{c}_3 = (-(\mathbf{a}+\mathbf{b}), (\mathbf{a}-\mathbf{b}))$, as shown in Fig. 5.2.4.2. The symbols $\widehat{c}_1, \widehat{c}_2, \widehat{c}_3$ then denote the same lattice, identical with the p-lattice with the conventional basis $(\mathbf{a}, \mathbf{b})$.

In the cases of the trigonal space-group types $P3_112$, D_3^3 (No. 151), $P3_121$, D_3^4 (No. 152), $P3_212$, D_3^5 (No. 153) and $P3_221$, D_3^6 (No. 154), and in the cases of the hexagonal space-group types $P6_122$, D_6^2 (No. 178) and $P6_522$, D_6^3 (No. 179), there exist two linear orbits with fixed parameter for which the sectional layer groups are monoclinic/rectangular with a c-centred lattice. The orientations of the unique axes of the respective monoclinic/rectangular groups are then defined by the choice of the conventional basis to which the Hermann–Mauguin symbol refers (*i.e.* by index in $\widehat{c}_1$, $\widehat{c}_2$ or $\widehat{c}_3$) and by the position of the twofold rotation in the symbol. In group types $P6_222$, D_6^4 (No. 180) and $P6_422$, D_6^5 (No. 181) there exist two linear orbits with fixed parameters for which the sectional layer groups are orthorhombic/rectangular with a c-centred lattice. The orientations of twofold axes of orthorhombic/rectangular groups in the section plane are again defined by the conventional bases $\widehat{c}_1, \widehat{c}_2$ or $\widehat{c}_3$. There are no other nontrivial orientation orbits in groups of

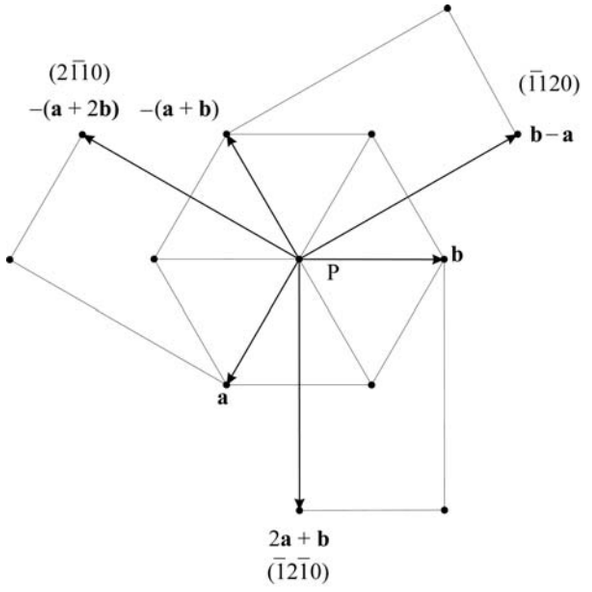

Fig. 5.2.4.3. Another choice of orthogonal basis vectors for a hexagonal lattice.

the Laue class $\bar{3}$ (C_{3i}) and no other orbits with fixed parameters in groups of the Laue class $6/m$ (C_{6h}).

Orientation orbits (01$\bar{1}$0) *and* ($\bar{1}$2$\bar{1}$0): These two orbits appear in all biaxial groups of the trigonal and hexagonal system, *i.e.* in groups of the Laue classes $\bar{3}m$ (D_{3d}) and $6/mmm$ (D_{6h}). We consider them together because corresponding scanning groups for pairs of orientations, one from each of these orbits, are related in the same way to their corresponding bases.

Hexagonal lattice. If the scanned group is trigonal with a primitive hexagonal lattice, the scanning group is monoclinic; if the scanned group is hexagonal, the scanning group is orthorhombic with lattice type *C*. Because of the choice of bases, the lattice is denoted by the letter *A* in the Hermann–Mauguin symbols of the scanning groups.

We choose the vector **c** of the hexagonal axis as the vector **a**′ for all orientations of these orbits. In addition we choose $\mathbf{b}' = \mathbf{a}$ and the scanning direction $\mathbf{d} = \mathbf{a} + 2\mathbf{b}$ for the orientation (01$\bar{1}$0), while for the orientation (2$\bar{1}\bar{1}$0), perpendicular to it, we choose $\mathbf{b}' = -(\mathbf{a} + 2\mathbf{b})$, $\mathbf{d} = \mathbf{a}$. Analogously, for the other pairs of mutually perpendicular orientations we choose: $\mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -(2\mathbf{a} + \mathbf{b})$ for the orientation ($\bar{1}$010); $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{d} = \mathbf{b}$ for the orientation ($\bar{1}$2$\bar{1}$0); $\mathbf{b}' = -(\mathbf{a} + \mathbf{b})$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation (1$\bar{1}$00); and $\mathbf{b}' = (\mathbf{b} - \mathbf{a})$, $\mathbf{d} = -(\mathbf{a} + \mathbf{b})$ for the orientation ($\bar{1}\bar{1}$20). Hence the scanning groups for the pairs of orientations (01$\bar{1}$0)/(2$\bar{1}\bar{1}$0), ($\bar{1}$010)/($\bar{1}$2$\bar{1}$0) and (1$\bar{1}$00)/($\bar{1}\bar{1}$20) are the same monoclinic or orthorhombic groups but the conventional basis vectors **b**′, **d** of one of them are replaced by −**d**, **b**′, respectively, for the second one. Again there are cases when the locations of scanning groups are different for different pairs of orientations, in which case the corresponding row splits into three subrows. To compare the geometry of the bases, consult and compare Figs. 5.2.4.2 and 5.2.4.3.

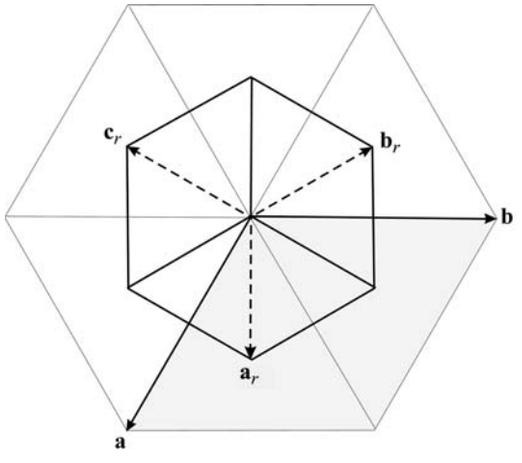

Fig. 5.2.4.4. The relationship between hexagonal and rhombohedral bases in the obverse setting.

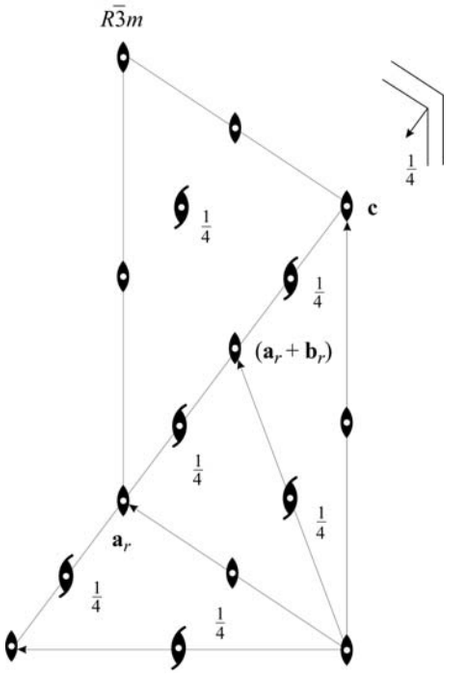

Fig. 5.2.4.5. The diagram of the scanning group $R\bar{3}m$ in the plane of orientation ($\bar{1}$2$\bar{1}$0) projected orthogonally along **b**.

Rhombohedral lattice. The resulting scanning groups are monoclinic of the *I*-centred type. The vectors of the rhombohedral basis $\mathbf{a}_r$, $\mathbf{b}_r$, $\mathbf{c}_r$ are related to vectors **a**, **b**, **c** of the hexagonal basis as follows:

$$\mathbf{a}_r = (2\mathbf{a} + \mathbf{b} + \mathbf{c})/3, \quad \mathbf{b}_r = (-\mathbf{a} + \mathbf{b} + \mathbf{c})/3,$$
$$\mathbf{c}_r = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3, \qquad (5.2.4.11)$$

as shown in Fig. 5.2.4.4, which corresponds to the obverse setting. In Figs. 5.2.4.5 and 5.2.4.6, we show the diagrams of the scanning groups in the plane of orientation ($\bar{1}$2$\bar{1}$0) for the groups $R\bar{3}m$, D^5_{3d} (No. 166) and $R\bar{3}c$, D^6_{3d} (No. 167), projected orthogonally along the direction of **b**. The vector $(\mathbf{a}_r + \mathbf{b}_r)$, whose projection is shown in both figures, is identical with the vector $(\mathbf{a}_r + \mathbf{b} + \mathbf{c})/2$ which is the *I*-centring vector of the monoclinic cell with conventional basis $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}_r$, $\mathbf{d} = \mathbf{b}$. The vector **b** plays the role of the scanning direction for orientation ($\bar{1}$2$\bar{1}$0) to which it is perpendicular (this is the case of monoclinic/orthogonal scanning). For the orientation ($\bar{1}$010), we choose the basis of the scanning group as $\mathbf{a} = \mathbf{c}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -\mathbf{a}_r$, and we get a monoclinic/inclined scanning.

One standard scanning table is given for each of the seven group types with a rhombohedral lattice because neither the bases of scanning groups nor their symbols change with the change from hexagonal to rhombohedral basis. None of the entries in the scanning tables needs to be changed with the exception of Bravais–Miller indices (*hkil*), which are replaced by corresponding Miller indices (*hkl*) as follows: (0001) is replaced

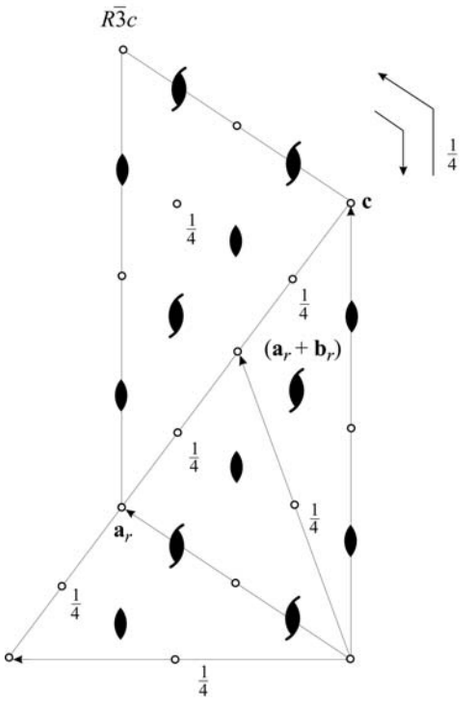

Fig. 5.2.4.6. The diagram of the scanning group $R\bar{3}c$ in the plane of orientation $(\bar{1}2\bar{1}0)$ projected orthogonally along **b**.

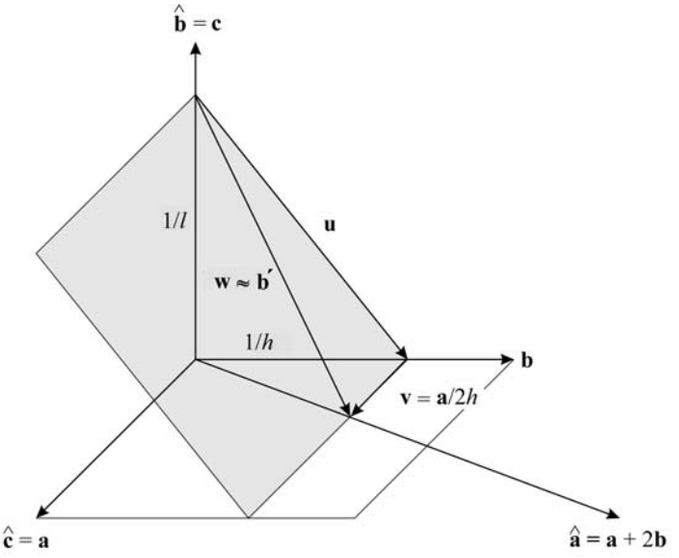

Fig. 5.2.4.7. Illustration of the transformation of Bravais–Miller indices in a hexagonal basis to Bravais indices in an auxiliary basis.

by (111), the set $(01\bar{1}0)$, $(\bar{1}010)$, $(1\bar{1}00)$ by $(11\bar{1})$, $(\bar{1}11)$, $(1\bar{1}1)$ and the set $(\bar{1}2\bar{1}0)$, $(\bar{1}\bar{1}20)$, $(2\bar{1}\bar{1}0)$ by $(01\bar{1})$, $(\bar{1}01)$, $(1\bar{1}0)$. The indices are given in parallel in the two columns for the designation of orientation orbits. To abbreviate expressions for vectors of the conventional bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of scanning groups, we express these vectors in terms of vectors of hexagonal basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and of vectors of rhombohedral basis $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$. To obtain the bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ in terms of vectors of the hexagonal basis, we substitute for vectors of the rhombohedral bases the combinations (5.2.4.11), to obtain them in terms of vectors of rhombohedral bases, we substitute for vectors of hexagonal bases the combinations

$$\mathbf{a} = \mathbf{a}_r - \mathbf{b}_r, \quad \mathbf{b} = \mathbf{b}_r - \mathbf{c}_r, \quad \mathbf{c} = \mathbf{a}_r + \mathbf{b}_r + \mathbf{c}_r, \qquad (5.2.4.12)$$

reciprocal to (5.2.4.11).

5.2.4.5.2. Inclined scanning, auxiliary tables

There are no orientation orbits with variable parameter and hence no auxiliary tables to the Laue class $\bar{3}$ (C_{3i}).

Orientation orbit $(mn\,\overline{m+n}\,0)$: This orbit appears in groups of the Laue class $6/m$ (C_{6h}), where it contains the three orientations $(mn\,\overline{m+n}\,0)$, $(\overline{m+n}\,mn0)$ and $(n\,\overline{m+n}\,m0)$; further, it appears in groups of the Laue class $6/mmm$ (D_{6h}), where it contains six orientations – to the three orientations we add their images generated by auxiliary axes or planes, which are the orientations $(nm\,\overline{m+n}\,0)$, $(\overline{m+n}\,nm0)$ and $(m\,\overline{m+n}\,n0)$. The choice of basis vectors for the scanning group of the first orientation $(mn\,\overline{m+n}\,0)$ is: $\mathbf{a}' = \mathbf{c}, \mathbf{b}' = n\mathbf{a} - m\mathbf{b}$ and $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$; as always in monoclinic/inclined scanning, the bases for other orientations are obtained by rotations around the principal axis [Laue class $6/m$ (C_{6h})] and by reflections in auxiliary planes [Laue class $6/mmm$ (D_{6h})], so that the scanning groups and the scanning are expressed by identical symbols in their respective bases.

For the particular values $m = 0$, $n = 1$ or $m = -1$, $n = 2$, the orientation orbit turns into a special orbit $(01\bar{1}0)$ or $(\bar{1}2\bar{1}0)$ with fixed parameters, respectively, for which the scanning group and hence the scanning is orthorhombic.

Orientation orbits $(0h\bar{h}l)$ and $(\bar{h}2h\bar{h}l)$: These two orbits include those orientations which contain the secondary or tertiary directions of the hexagonal system. Both orbits exist in the Laue classes $\bar{3}m$ (D_{3d}) and $6/mmm$ (D_{6h}); the orbit $(0h\bar{h}l)$ appears in the arithmetic classes $321P$, $3m1P$, $\bar{3}m1P$ and $32R$, $3mR$, $\bar{3}mR$, where it contains further the two orientations $(\bar{h}0hl)$ and $(h\bar{h}0l)$; the orbit $(\bar{h}2h\bar{h}l)$ appears in the arithmetic classes $312P$, $31mP$ and $\bar{3}1mP$, where it contains the two other orientations $(\overline{hh}2hl)$, $(2h\overline{hh}l)$: both orbits appear in all groups of the Laue class $6/mmm$ (D_{6h}) where they contain additional triplets of orientations: $(0h\overline{hl})$, $(\bar{h}0h\bar{l})$ and $(h\bar{h}0\bar{l})$ in the first case and $(\bar{h}2h\overline{hl})$, $(\overline{hh}2h\bar{l})$ and $(2h\overline{hh}l)$ in the second case.

Transformation of Bravais–Miller indices: hexagonal axes. The orientations $(0h\bar{h}l)$ are specified by Bravais–Miller indices with reference to the hexagonal basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ through integers h, l. To find their Miller indices $(mn0)$ with reference to auxiliary bases $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}})$, we consider a vector $\mathbf{w} = \mathbf{u} + \mathbf{v} \approx [l(\mathbf{a} + 2\mathbf{b}) - 2h\mathbf{c}]$ as shown in Fig. 5.2.4.7. This vector is proportional to a vector $\mathbf{b}'$, which is used as a vector of the conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of the scanning group in both centring types P and R. Vector $\mathbf{b}'$ is defined as $\mathbf{b}' = n\hat{\mathbf{a}} - m\hat{\mathbf{b}}$, where $\hat{\mathbf{a}} = \mathbf{a} + 2\mathbf{b}$ for both the centring types P and R, while $\hat{\mathbf{b}} = \mathbf{c}$ for the centring type P and $\hat{\mathbf{b}} = \mathbf{c}_r$ for the centring type R.

The proportionality relations therefore read for the centring type P

$$l(\mathbf{a} + 2\mathbf{b}) - 2h\mathbf{c} \approx n(\mathbf{a} + 2\mathbf{b}) - m\mathbf{c}, \qquad (5.2.4.13)$$

from which we express n, m through h, l as follows:

$$l \text{ odd } \Rightarrow n = l, m = 2h; \quad l \text{ even } \Rightarrow n = l/2, m = h.$$

In the case of the centring type R, we have

$$\begin{aligned}\mathbf{b}' &= n(\mathbf{a} + 2\mathbf{b}) - m(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3 \\ &= (n + m/3)(\mathbf{a} + 2\mathbf{b}) - m\mathbf{c}/3,\end{aligned}$$

so that the proportionality relation reads

$$l(\mathbf{a}+2\mathbf{b})-2h\mathbf{c}\approx(n+m/3)(\mathbf{a}+2\mathbf{b})-(m/3)\mathbf{c}. \qquad (5.2.4.14)$$

Comparing the coefficients, we obtain that the pair (n, m) must be proportional to the pair $(l-2h, 6h)$, from which we express n, m through h, l as follows:

$$l \text{ odd } \Rightarrow n=l-2h, m=6h; \quad l \text{ even } \Rightarrow n=l/2-h, m=3h.$$

For the orientation orbit $(\bar{h}2h\bar{h}l)$, we obtain the proportionality relation by comparing the proportional vectors $\mathbf{b}'=n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}=n\mathbf{b}-m\mathbf{c}$ and $l\mathbf{b}-2h\mathbf{c}$, which leads again to the relations

$$l \text{ odd } \Rightarrow n=l, m=2h; \quad l \text{ even } \Rightarrow n=l/2, m=h.$$

The relations between indices h, l and m, n are, as usual, recorded under each orbit in a row across the table.

The orientation orbits $(0h\bar{h}l)$ and $(\bar{h}2h\bar{h}l)$ turn into the special orbits $(01\bar{1}0)$ and $(\bar{1}2\bar{1}0)$ with fixed parameter for the special values $h=1$, $l=0$, and their symmetry increases to orthorhombic for groups of the Laue class $6/mmm$ (D_{6h}). In groups of the Laue class $\bar{3}m$ (D_{3d}), the symmetry of these orbits remains monoclinic but the scanning changes from monoclinic/inclined to monoclinic/orthogonal.

Rhombohedral axes. Auxiliary tables for the five group types with a rhombohedral lattice are given in a compact manner for all three arithmetic classes. Neither auxiliary nor conventional (in the sense of the convention for scanning groups, see Section 5.2.2.3) bases of scanning groups change. The orientations of the orbit are expressed by Bravais–Miller indices in the hexagonal basis and these are transformed to Miller indices $(mn0)$ with reference to the auxiliary basis as shown above. In the rhombohedral basis, we describe orientations of the orbit by Miller indices (hhl). The integers h, l here are considered independently of the same letters in Bravais–Miller indices. To transform them into Miller indices with reference to the auxiliary basis, we take into account that the vector $\mathbf{w}$ from Fig. 5.2.4.7 is proportional to $l(\mathbf{a}_r+\mathbf{b}_r)-2h\mathbf{c}_r$ as well as to $n(\mathbf{a}_r+\mathbf{b}_r+\mathbf{c}_r)-m\mathbf{c}_r=n(\mathbf{a}_r+\mathbf{b}_r)+(n-m)\mathbf{c}_r$. Comparing coefficients at $(\mathbf{a}_r+\mathbf{b}_r)$ and $\mathbf{c}_r$ we obtain

$$l \text{ odd } \Rightarrow n=l, m=2h+l; \quad l \text{ even } \Rightarrow n=l/2, m=h+l/2.$$

The reference table is given as a common table for consideration in hexagonal or rhombohedral axes. It is also common for all five group types with rhombohedral lattice for which this type of orientation orbit occurs.

5.2.4.6. Cubic system

The character of scanning is again different for groups of the geometric classes 23 (T) and $m\bar{3}$ (T_h) with no fourfold axes and for groups of the geometric classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h) which contain fourfold axes.

The threefold axis along the direction [111] passes through the origin in all cubic groups, including the cases when two origin choices are used. Rotations around this axis therefore transform the coordinate system in such a way that the conjugate scanning groups, linear orbits and sectional layer groups are expressed in the same way in the respective coordinate systems.

5.2.4.6.1. Orthogonal scanning, standard tables

Orientation orbit (001): This orientation orbit contains the orientations (001), (100) and (010). It appears in all cubic groups and it leads to orthorhombic scanning groups in the case of space groups of the classes 23 (T), $m\bar{3}$ (T_h) and to tetragonal scanning groups in the case of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The conventional bases of the scanning groups for the orientation (001) are chosen as $\mathbf{a}'=\mathbf{a}$, $\mathbf{b}'=\mathbf{b}$, $\mathbf{d}=\mathbf{c}$ for all cases with the exception of F-centred types of groups of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The centring types P, I and F remain the same for orthorhombic scanning groups, *i.e.* for the classes 23 (T) and $m\bar{3}$ (T_h), and for the P and I types of tetragonal scanning groups which apply to the classes 23 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The F-centred type for the latter classes turns into I-centred tetragonal scanning groups with the conventional basis $\mathbf{a}'=(\mathbf{a}-\mathbf{b})/2$, $\mathbf{b}'=(\mathbf{a}+\mathbf{b})/2$, $\mathbf{d}=\mathbf{c}$ for the orientation (001).

For the remaining two orientations (100) and (010), we obtain the bases by the cyclic permutations $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ and $\mathbf{a}\rightarrow\mathbf{c}\rightarrow\mathbf{b}\rightarrow\mathbf{a}$, respectively, which correspond to rotations 3 and 3^2 around the threefold axis [111].

Orientation orbit (110): This orbit occurs only in groups of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). It consists of the orientations (110), $(1\bar{1}0)$, (011), $(01\bar{1})$, (101) and $(\bar{1}01)$. The scanning groups are orthorhombic in all cases. We choose the conventional basis of the scanning group as $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=(\mathbf{a}-\mathbf{b})$, $\mathbf{d}=(\mathbf{a}+\mathbf{b})$ for the orientation (110) and as $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=(\mathbf{a}+\mathbf{b})$, $\mathbf{d}=(\mathbf{b}-\mathbf{a})$ for the orientation $(1\bar{1}0)$ for the P- and I-centred cases. The corresponding scanning groups are orthorhombic of the centring types A and F, respectively. For the original F-centring, we choose the conventional basis of orthorhombic scanning groups as $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=(\mathbf{a}-\mathbf{b})/2$, $\mathbf{d}=(\mathbf{a}+\mathbf{b})/2$ for the orientation (110) and as $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=(\mathbf{a}+\mathbf{b})/2$, $\mathbf{d}=(\mathbf{a}-\mathbf{b})/2$ for the orientation $(1\bar{1}0)$, which results in I-centred orthorhombic scanning groups.

The bases for the scanning groups corresponding to the orientations (011) and $(01\bar{1})$ are obtained respectively by the cyclic permutation $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ and the bases of scanning groups for the orientations (101) and $(\bar{1}01)$ by the cyclic permutation $\mathbf{a}\rightarrow\mathbf{c}\rightarrow\mathbf{b}\rightarrow\mathbf{a}$, which again corresponds to the threefold rotations 3 and 3^2 around the [111] axis. Accordingly, the scanning groups, linear orbits and sectional layer groups are the same with reference to respective bases for the orientations (110), (011) and (101) as well as for the orientations $(1\bar{1}0)$, $(01\bar{1})$ and $(\bar{1}01)$. In some cases, there is also no difference between the two triplets of orientations and one row describes the scanning for all six orientations. In other cases, owing to fourfold screw axes, the scanning groups are shifted and the row splits into two subrows.

Orientation orbit (111): This orbit with orientations (111), $(\bar{1}\bar{1}1)$, $(1\bar{1}\bar{1})$ appears in all cubic groups and the respective scanning groups are trigonal with a rhombohedral lattice. The following abbreviated symbols are used for vectors of the cube diagonals:

$$\boldsymbol{\tau}=(\mathbf{a}+\mathbf{b}+\mathbf{c}), \quad \boldsymbol{\tau}_1=(\mathbf{a}-\mathbf{b}-\mathbf{c}),$$
$$\boldsymbol{\tau}_2=(-\mathbf{a}+\mathbf{b}-\mathbf{c}), \quad \boldsymbol{\tau}_3=(-\mathbf{a}-\mathbf{b}+\mathbf{c})$$

in directions [111], $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$ and $[\bar{1}\bar{1}1]$, see Fig. 5.2.4.8. The latter three vectors are obtained from the vector $\boldsymbol{\tau}$ by the action of twofold axes as follows: $2_z\boldsymbol{\tau}=\boldsymbol{\tau}_3$, $2_x\boldsymbol{\tau}=\boldsymbol{\tau}_1$, $2_y\boldsymbol{\tau}=\boldsymbol{\tau}_2$. The rhombohedral unit cells of the scanning groups corresponding to the orientation (111) and for the P-, I- and F-centring types of original cubic groups are shown in Figs. 5.2.4.9(a), 5.2.4.10(a) and 5.2.4.11(a), respectively. Eight conventional cubic cells surrounding the origin are shown in each of the figures to display the hexagonal lattice in the plane corresponding to the orientation (111) and passing through the origin. The projections of these situations along the cube diagonal $\mathbf{d}$ onto this plane are

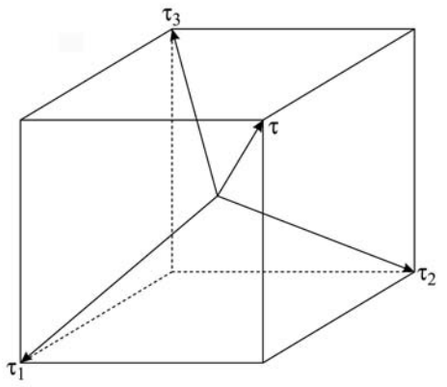

Fig. 5.2.4.8. Vectors along the main cubic axes.

depicted in Figs. 5.2.4.9(*b*), 5.2.4.10(*b*) and 5.2.4.11(*b*), respectively. In these figures, the areas that represent the choice of the hexagonal unit cell in the plane as used for scanning groups are shaded. The scanning direction is chosen along the cube diagonal [111]. Notice that the periodicity of the corresponding hexagonal lattice in this direction equals $\mathbf{d} = \boldsymbol{\tau}$ for *P*- and *F*-centred cubic groups, while for the *I*-centred groups the periodicity is $\mathbf{d} = \boldsymbol{\tau}/2$. The choice of bases of the scanning groups corresponds to the obverse setting of the rhombohedral basis vectors with respect to hexagonal bases. The scanning for the direction [111] can be then copied from the scanning of trigonal groups with a rhombohedral lattice.

The remaining three orientations $(\overline{1}\overline{1}1)$, $(1\overline{1}\overline{1})$ and $(\bar{1}1\bar{1})$ are obtained by application of twofold rotations 2_z, 2_x and 2_y, respectively. Using these rotations, we obtain the scanning data in a compact way for all four orientations. Again, in certain cases,

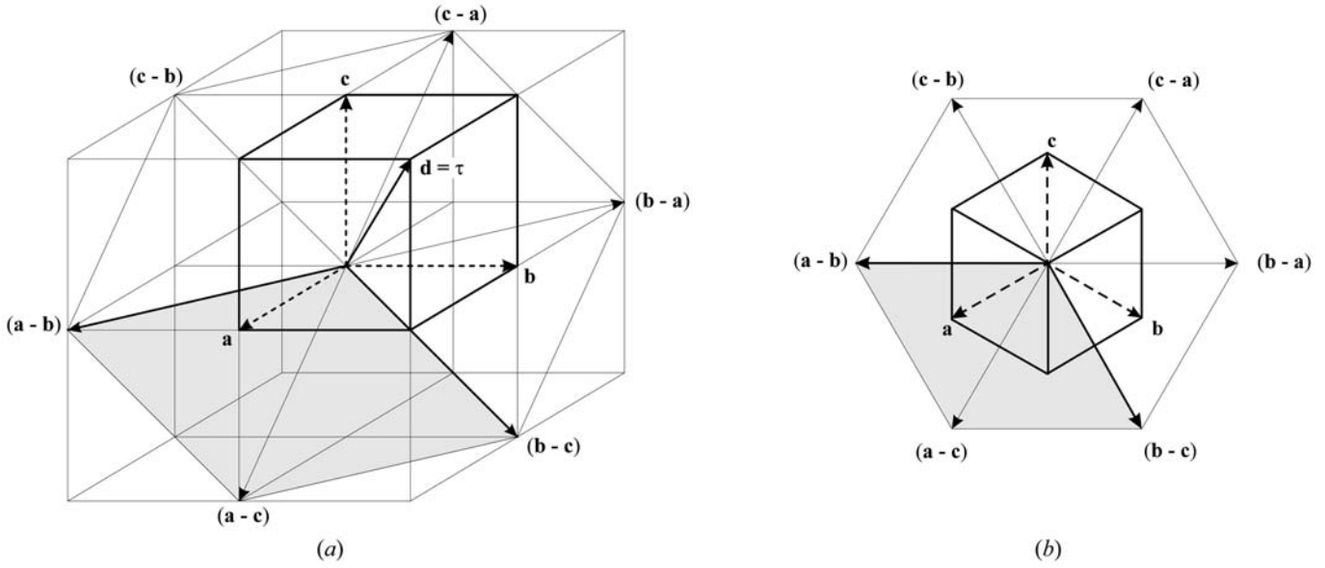

Fig. 5.2.4.9. The cubic scanning for orientation (111) in the case of cubic groups with a *P* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

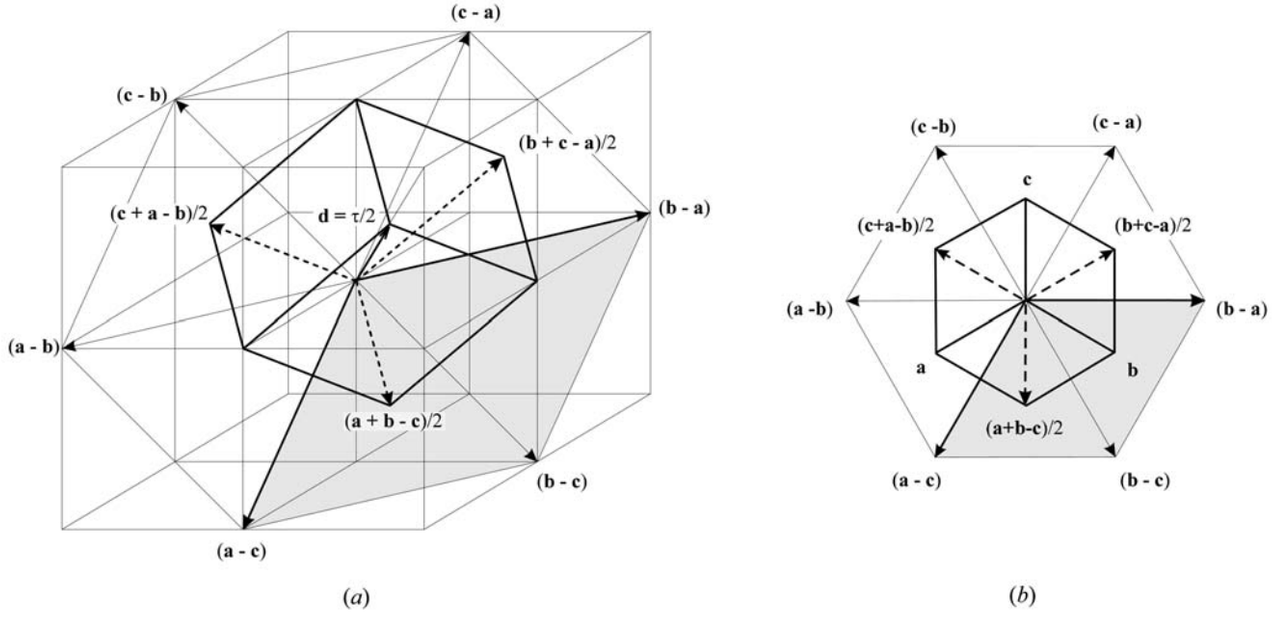

Fig. 5.2.4.10. The cubic scanning for orientation (111) in the case of cubic groups with an *I* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

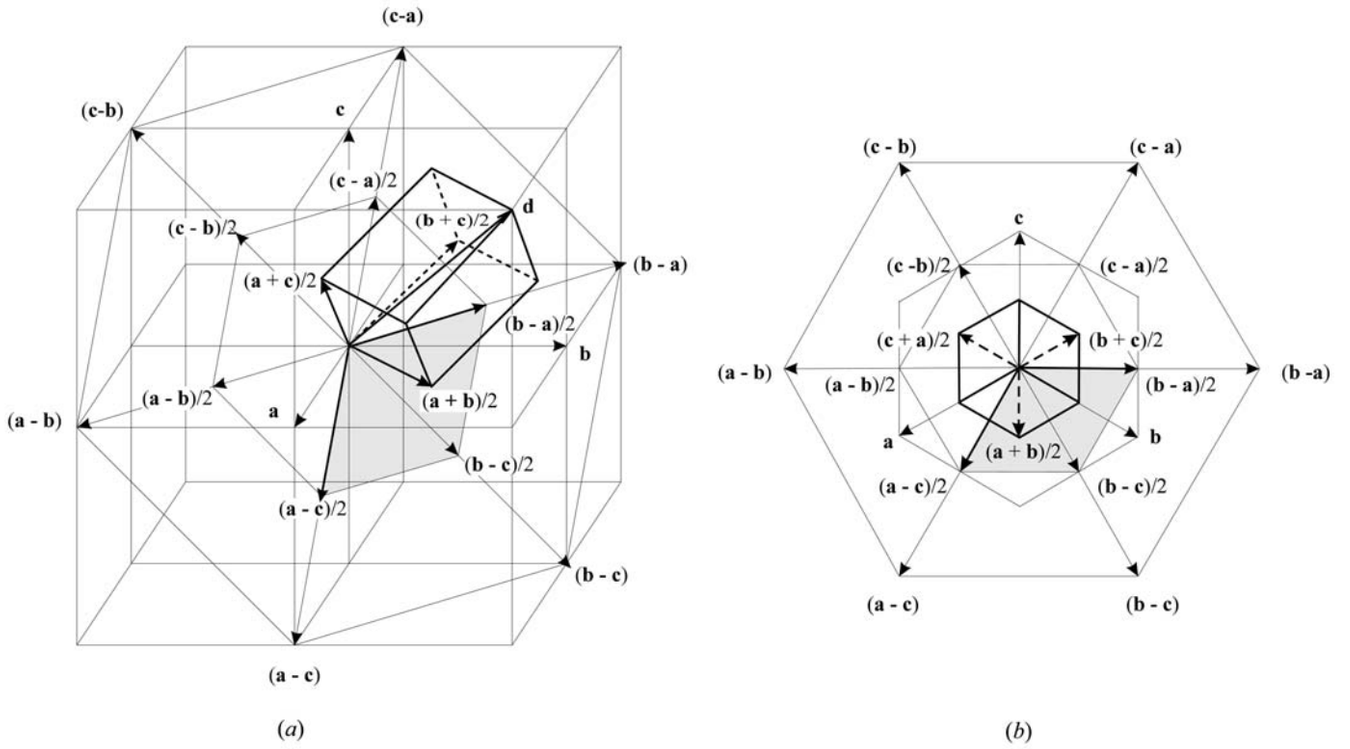

Fig. 5.2.4.11. The cubic scanning for orientation (111) in the case of cubic groups with an *F* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

the data are the same with respect to the rotated coordinate systems; then one row describes all orientations. In other cases, the data refer to shifted coordinate systems. The shifts along the scanning direction, if they are the same for all orientations, are taken into account by recalculating the levels of the linear orbits. The shifts in planes ($\mathbf{a}'$, $\mathbf{b}'$) are, however, used to refer to different origins.

5.2.4.6.2. Inclined scanning, auxiliary tables

Orientation orbit (*mn*0): Orientations of this orbit contain one of the three main cubic axes and are divided into three subsets corresponding to these axes for which the bases are separated by horizontal lines in the tables of orientation orbits and auxiliary bases. The orbit contains six orientations in groups of the Laue class $m\bar{3}$ (T_h) and 12 orientations in groups of the Laue class $m\bar{3}m$ (O_h). The orbit turns into a special orbit with fixed parameters for the special values $m = 1, n = 0$ in groups of both the Laue classes $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h). The scanning changes from monoclinic/inclined to orthorhombic in the Laue class $m\bar{3}$ (T_h), to tetragonal in the Laue class $m\bar{3}m$ (O_h). The symmetry of the orientation also increases to orthorhombic for special values $m = 1$, $n = 1$ in groups of the Laue class $m\bar{3}m$ (O_h).

The choice of bases for the three subsets is the same as in orthorhombic groups, where the orientations of subsets are separated into three different orbits and the auxiliary bases are expressed in terms of vectors of the conventional cubic basis for the centring types *P* and *I*. For the centring type *F*, the Miller indices differ in the original and auxiliary basis. In this case, we express the Miller indices with reference to the original basis as (*hk*0) and relate them to Miller indices (*mn*0) with reference to the auxiliary bases. These relations are the same as in the case of *F*-centring in orthorhombic groups, see relations (5.2.4.2) and (5.2.4.3).

Orientation orbit (*hhl*): The orbit contains 12 orientations which divide into three subsets corresponding to the three main cubic axes. In each of the subsets, one of the vectors of the conventional cubic basis is chosen as the vector $\widehat{\mathbf{b}}$ of the auxiliary basis. The orientations of the subsets are separated by horizontal lines across the table. The first subset corresponds to the vector **c** of the cubic basis and the orientations in this subset are the same as in the (*hhl*) orbit for tetragonal groups of the Laue class $4/mmm$ (D_{4h}). The orientations within each subset are further divided into two pairs of orientations to which correspond two different unique axes of the monoclinic scanning group. These subsets are again separated by horizontal lines across the last two columns. For the centring types *P* and *I* and for the first subset of orientations, the description of orientations and bases coincides with the description of the orbit (*hhl*) in tetragonal groups of the Laue class $4/mmm$ (D_{4h}) and centring types *P* and *I*, including the choice of auxiliary and conventional bases of scanning groups and relations between Miller indices *h*, *l* and *m*, *n*. For the other subsets of orientations, the data in tables are obtained by the cyclic permutation of vectors **a**, **b** and **c**.

For the centring type *F*, orientation (*hhl*), we choose the auxiliary basis of the scanning group with the unique axis vectors $\widehat{\mathbf{c}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} + \mathbf{b})/2$, while for the orientation ($h\bar{h}l$), we choose $\widehat{\mathbf{c}} = (\mathbf{a} + \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$. The bases for the remaining orientations are again obtained by the cyclic permutation of vectors of the conventional cubic basis.

Transformation of Miller indices: The straight line in which a plane (*hhl*) intersects with the plane ($1\bar{1}0$) has the direction of a vector $(\mathbf{a} + \mathbf{b})/2h - \mathbf{c}/l$ or of the vector $\mathbf{b}' = n\widehat{\mathbf{a}} - m\mathbf{c} = n(\mathbf{a} + \mathbf{b})/2 - m\mathbf{c}$. As these two vectors can differ only by a numerical factor, the pair $(2m, n)$ must be proportional to the pair (h, l) and we obtain the relations

$$h \text{ odd } \Rightarrow m = h, n = 2l; \quad h \text{ even } \Rightarrow m = h/2, n = l,$$

recorded at the bottom row of the orientation-orbit table for the centring type *F*.

For the special values $h = 1, l = 0$, this orbit turns into an orbit (110) with fixed parameters and an orthorhombic scanning group.

5.2.5. Applications

5.2.5.1. Layer symmetries in crystal structures

The following two examples show the use of layer symmetries in the description of crystal structures.

Example 1

Fig. 5.2.5.1 shows the crystal structure of cadmium iodide, CdI_2. The space group of this crystal is $P\bar{3}m1$, D_{3d}^3 (No. 164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI_2 structure is:

A	C	B	C
I	Cd	I	void

From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

The plane at height $0\mathbf{c}$ contains cadmium ions. This plane defines the orbit of planes of orientation (0001) located at points $P + n\mathbf{c}$, where $n \in Z$ (Z is the set of all integers). All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $\frac{1}{2}\mathbf{c}$ defines the orbit of planes of orientation (0001) located at points $P + (n + \frac{1}{2})\mathbf{c}$, where $n \in Z$. All these planes lie midway between A and B layers of iodine ions with the B layer below, the A layer above the plane. They contain only voids.

The planes at levels $\frac{1}{4}\mathbf{c}$ and $\frac{3}{4}\mathbf{c}$ contain B and A layers of iodine ions, respectively. These planes and all planes produced by translations $n\mathbf{c}$ from them belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

Example 2

The space group of cadmium chloride, $CdCl_2$, is $R\bar{3}m$, D_{3d}^5 (No. 166). Fig. 5.2.5.2 shows the structure of $CdCl_2$ in its triple hexagonal cell. The anions form a cubic close packing of spheres and the cations occupy half of the octahedral holes of each alternate layer. In close-packing notation, the $CdCl_2$ structure is:

A	C	B	A	C	B	A	C	B	A	C	B
Cl	Cd	Cl	void	Cl	Cd	Cl	void	Cl	Cd	Cl	void

We choose the origin at a cadmium ion and the hexagonal basis vectors **a**, **b** as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}$, $\frac{1}{6}\mathbf{c}$, $\frac{1}{3}\mathbf{c}$, $\frac{1}{2}\mathbf{c}$, $\frac{2}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ have a sectional layer group of the type $p\bar{3}m1$ (L72) and at any other height have a sectional layer group of the type $p3m1$ (L69).

The scanning table also specifies the location of the sectional layer groups. The position along the c axis, where the basis vector $\mathbf{c} = \mathbf{d}$ specifies the scanning direction, is given by fractions of **d** or by $s\mathbf{d}$ in the case of a general position. At the heights $0\mathbf{c}$ and $\frac{1}{2}\mathbf{c}$, the sectional layer group is the group $p\bar{3}m1$ (L72), while at the heights $\frac{1}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(\mathbf{a} + 2\mathbf{b})/3]$ (L72), and at the heights $\frac{2}{3}\mathbf{c}$ and $\frac{1}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(2\mathbf{a} + \mathbf{b})/3]$, (L72), where the vectors in brackets mean the shift of the group $p\bar{3}m1$ in space. The planes at the heights $0\mathbf{d}$, $\frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}$ belong to one translation orbit and the layers contain cadmium ions which are shifted relative to each other by the vectors $(\mathbf{a} + 2\mathbf{b})/3$ and $(2\mathbf{a} + \mathbf{b})/3$. The planes at the heights $\frac{1}{2}\mathbf{d}$, $\frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}$ contain the voids and are located midway between layers of chlorine ions; they belong to another linear orbit and again are shifted relative to each other by the vectors $(\mathbf{a} + 2\mathbf{b})/3$ and $(2\mathbf{a} + \mathbf{b})/3$.

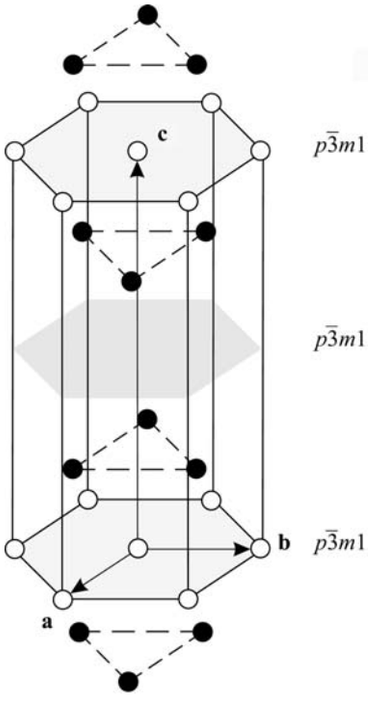

Fig. 5.2.5.1. The structure of cadmium iodide, CdI_2. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

5.2.5.2. Interfaces in crystalline materials

The scanning for the sectional layer groups is a procedure which finds applications in the theory of *bicrystals* and their *interfaces*. The first of these two terms was introduced in the study of grain boundaries (Pond & Bollmann, 1979; Pond & Vlachavas, 1983; Vlachavas, 1985; Kalonji, 1985). An *ideal bicrystal* is understood to be an aggregate of two semi-infinite crystals of identical structure, meeting at a common planar boundary called the *interface*, where one of the structures, occupying half-space on one side of the interface, is misoriented and/or displaced relative to the other structure occupying the other half-space. The word interface is a synonym for a boundary and interfaces considered here are *homophase interfaces*, in contrast with *heterophase interfaces*, where the two structures are different (Sutton & Balluffi, 1995).

An independent study of domain and twin boundaries (Janovec, 1981; Zikmund, 1984) resulted in a terminology parallel to that of the *bicrystallography*. The basic concept here is the *domain twin*, which is technically a particular case of a bicrystal. In this section, we use the terminology of bicrystals, giving the terminology of domain twins, used in the next section, parenthetically.

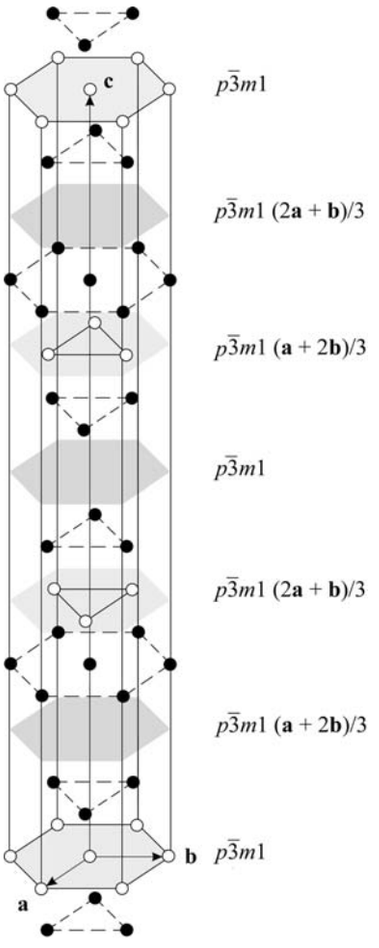

Fig. 5.2.5.2. The structure of cadmium chloride, $CdCl_2$. The section planes of two orbits in special positions are distinguished by shading. Notice the different location of the sectional layer groups on different levels for the same orbit. The figure is drastically elongated in the *c* direction to exhibit the layer symmetries.

In both cases, the aim of the analysis is to determine the symmetry group of a bicrystal (domain twin), corresponding to a certain orientation and location of the interface (domain wall or twin boundary), which is a certain layer group.

The bicrystal (domain twin) is a conceivable real structure in space!

In the first step of the analysis, one constructs a *dichromatic complex* or *pattern* [(*unordered*) *domain pair*].

The dichromatic complex (domain pair) is not a real structure!

It is an abstract construction, a superposition of two infinite crystals which have the same structure, orientation and/or location as the two semi-infinite crystals of the bicrystal (domain twin) when extended to infinity. The two components are referred to as *black and white crystals* or *variants* (*single domain states*).

The symmetry group $\mathcal{J}$ of the dichromatic complex (domain pair) is the group of those Euclidean motions which either leave both black and white crystals (domain states) invariant or which exchange them. Planes of various orientations and locations, representing the interface, are then considered as transecting the dichromatic complex (domain pair). To each such plane there corresponds a sectional layer group $\bar{\mathrm{J}}$, the elements of which leave invariant the dichromatic pattern (domain pair) and the plane. A bicrystal (domain twin) is obtained by deleting from one side of the plane the atoms of one of the components of the dichromatic pattern (single domain states) and the atoms of the second component (single domain state) from the other side of the plane. The symmetry of the bicrystal (domain twin) is a layer group which contains those elements of the sectional layer group of the dichromatic pattern (domain pair) that satisfy one of the following two conditions:

(i) elements that leave invariant both the black and white crystals (both single domain states) and the normal to the plane;

(ii) elements that exchange the black and white crystals (single domain states) and invert the normal to the plane.

Example

Consider the bicrystal consisting of two face-centred cubic crystals misoriented by a rotation of 36.9° about the [001] direction. The corresponding dichromatic complex is shown in Fig. 5.2.5.3. The symmetry group of the complex is the space group $I4/mmm$, D_{4h}^{17} (No. 139).

Vlachavas (1985) has tabulated the symmetries of bicrystals arising when the above dichromatic complex is transected with planes of various orientations and locations. For planes of the orientation (001), given with reference to the tetragonal coordinate system shown in Fig. 5.2.5.3, Vlachavas lists

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Symmetry group of the bicrystal	$p422$	$p42_12$	$p411$

The position of the plane is given in terms of a fraction of the basis vector of the tetragonal *c* axis. The '*p*' in the symbol of the symmetry groups of the bicrystal denotes all translations in the (001) plane.

From the subtable for the space group $I4/mmm$, D_{4h}^{17} (No. 139) in the scanning tables, Part 6, one finds

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Sectional layer group	$p4/mmm$	$p4/mmm$	$p4mm$

The symmetry group of the bicrystal is that subgroup of the corresponding sectional layer group consisting of all elements that satisfy one of the two conditions given above. For example, for the plane at position '0', the sectional layer group is $p4/mmm$ (L61). None of the mirror planes satisfies either of the conditions. The mirror plane perpendicular to [001] inverts the normal to the plane but leaves invariant both black and white crystals. The mirror planes perpendicular to [001] and [010] leave the normal to the plane invariant, but exchange the black and white crystals. The fourfold rotation satisfies condition (i), and the twofold rotations about auxiliary axes satisfy condition (ii). Consequently, from the sectional layer groups $p4/mmm$ (L61), $p4/nmm$ (L64) and $p4mm$ (L55) one obtains the respective symmetries of the bicrystal with different locations of interfaces: $p422$ (L53), $p42_12$ (L54) and $p4$ (L49), as listed by Vlachavas.

5.2.5.3. The symmetry of domain twins and domain walls

The symmetry of domain twins with planar coherent domain walls and the symmetry of domain walls themselves are also described by layer groups (see *e.g.* Janovec *et al.*, 1989), from

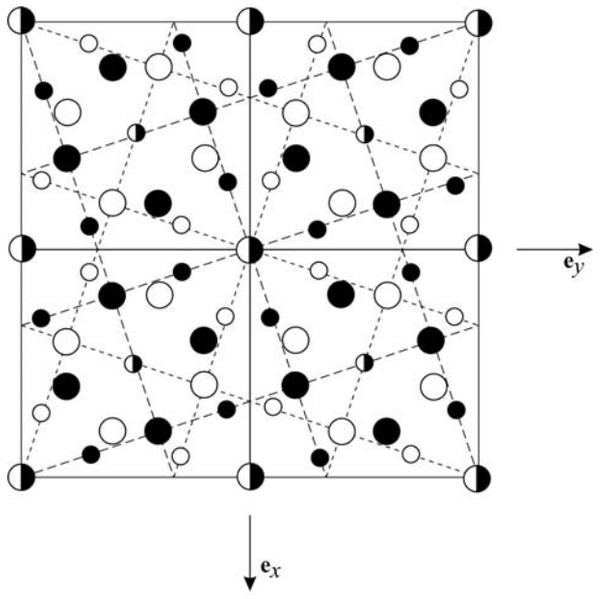

Fig. 5.2.5.3. A classical example of a bicrystal (Vlachavas, 1985).

which conclusions about the structure and tensorial properties of the domain walls can be deduced. The derivation of the layer symmetries of twins and domain walls is again facilitated by the scanning tables. As shown below, the symmetry of a twin is in general expressed through four sectional layer groups, where the central plane of the interface is considered as the section plane of an ordered and unordered domain pair. The relations between the symmetries and possible conclusions about the structure of the wall will be illustrated by an analysis of a domain twin in univalent mercurous halide (calomel) crystals.

A *twin* is a particular case of a bicrystal in which the relative orientation and/or displacement of the two components is not arbitrary; it is required that the operation that sends one of the components to the other is crystallographic. A *domain twin* is a special case where the structures S_1 and S_2 of the two components (*domains*) are distortions of a certain *parent* structure S, the symmetry of which is a certain space group $\mathcal{G}$, called the *parent group*. The parent structure S is either a real structure, the distortions of which are due to a structural phase transition, or it is a hypothetical structure. If the symmetry of one of the distorted structures S_1 is $\mathcal{F}_1$, then, from the coset decomposition

$$\mathcal{G} = \mathcal{F}_1 \cup g_2\mathcal{F}_1 \cup \ldots \cup g_p\mathcal{F}_1 \qquad (5.2.5.1)$$

we obtain $p = [\mathcal{G} : \mathcal{F}_1]$ equivalent distorted structures $\mathsf{S}_i = g_i\mathsf{S}_1$, $i = 1, 2, \ldots, p$, with symmetries $\mathcal{F}_i = g_i\mathcal{F}_1 g_i^{-1}$ which form a set of conjugate subgroups of $\mathcal{G}$.

Hence, a domain twin is always connected with a certain symmetry descent from a space group $\mathcal{G}$ to a set of conjugate subgroups $\mathcal{F}_i$. The distorted structures S_i are called the *single domain states*. A domain twin consists of two semi-infinite regions (half-spaces), called *domains*, separated by a planar interface called the *central plane*. The structures at infinite distance from this plane coincide with the domain states. The structure in the vicinity of the central plane is called the *domain wall*. The aim of the symmetry analysis is to determine the possible structure of the domain wall.

Basic theory: We consider a domain twin in which the domains are occupied by single domain states S_1 and S_2. To define the twin uniquely, we first observe that Miller indices (*hkl*) or corresponding normal $\mathbf{n}$ to the interface (central plane of the domain wall) define not only the orientation $V(\mathbf{a}', \mathbf{b}')$ of the wall but also its *sidedness*, so that one can distinguish between the two half-spaces. The normal $\mathbf{n}$ points from one of the half-spaces to the other while $-\mathbf{n}$ points in the opposite direction. The twin is then defined uniquely by the symbol $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2) = (\mathsf{S}_1|(hkl); s\mathbf{d}|\mathsf{S}_2)$, which means that the domains are separated by the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ of orientation $V(\mathbf{a}', \mathbf{b}')$ and location $s\mathbf{d}$, where $\mathbf{d}$ is the scanning vector. The symbol also specifies that the normal $\mathbf{n}$ points from the half-space occupied by domain state S_1 to the half-space occupied by domain state S_2.

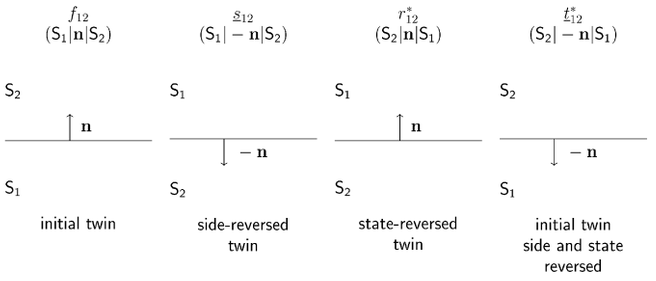

Fig. 5.2.5.4. The four types of operations on a twin.

Now we consider the changes of the twin under the action of those isometries which leave the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ invariant. The action of such an isometry g on the twin is expressed by $g(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2) = (g\mathsf{S}_1|\widehat{g}\mathbf{n}|g\mathsf{S}_2)$, where $\widehat{g}$ is the *linear constituent* of the isometry g and $\widehat{g}\mathbf{n} = \pm\mathbf{n}$. Among these isometries, there are in general two kinds which define the symmetry of the twin and two which reverse the twin. The symbols for these four kinds of operations, their action on the initial twin $(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2)$, their graphical representation and the names of the resulting twins are as shown in Fig. 5.2.5.4.

An auxiliary notation has been introduced in which an asterisk labels operations that exchange the domain states and an underline labels operations that change the normal to the plane of the wall. To avoid misinterpretation (the symbolism is similar to that of the symmetry–antisymmetry groups), let us emphasize that neither the asterisk nor the underline have any meaning of an operation; they are just suitable labels which can be omitted without changing the meaning of general or specific symbols of the isometries. Operations with these labels mean the same as if the labels are dropped.

The operations f_{12} leave invariant the normal $\mathbf{n}$ as well as the states S_1 and S_2. Such operations are called the *trivial symmetry operations of a domain twin* and they constitute a certain layer group $\widehat{\mathsf{F}}_{12}$. The $\underline{t}^*_{12}$ exchange the half-spaces because they invert the normal $\mathbf{n}$ and at the same time they exchange the domain states S_1 and S_2. As a result they leave the twin invariant, changing only the direction of the normal. These operations are called the *nontrivial symmetry operations of a domain twin*. If $\underline{t}^*_{12}$ is one such operation, then all these operations are contained in a coset $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$. Operations $\underline{s}_{12}$, called *the side-reversing operations*, exchange the half-spaces, leaving the domain states S_1 and S_2 invariant, and operations r^*_{12}, called *the state-reversing operations*, exchange the domain states S_1 and S_2, leaving the half-spaces invariant.

The symmetry group $\mathsf{T}(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$, or in short T_{12}, of the twin $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$ can therefore be generally be expressed as

$$\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_{12}, \qquad (5.2.5.2)$$

where $\widehat{\mathsf{F}}_{12}$ is a group of all trivial symmetry operations and $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$ is the coset of all nontrivial symmetry operations of the twin.

The group T_{12} is a layer group which can be deduced from four sectional layer groups of two space groups which describe the symmetry of two kinds of domain pairs formed from the domain states S_1 and S_2 (Janovec, 1972):

An *ordered domain pair* $(\mathsf{S}_1, \mathsf{S}_2) \neq (\mathsf{S}_2, \mathsf{S}_1)$ is an analogue of the dichromatic complex in which we keep track of the two components. The symmetry group of this pair must therefore leave invariant both domain states and is expressed as the intersection

$$\mathcal{F}_{12} = \mathcal{F}_1 \cap \mathcal{F}_2 = \mathcal{F}_1 \cap g_{12}\mathcal{F}_1 g_{12}^{-1} \qquad (5.2.5.3)$$

of symmetry groups $\mathcal{F}_1$ and $\mathcal{F}_2 = g_{12}\mathcal{F}_1 g_{12}^{-1}$ of the respective single domain states S_1 and S_2, where g_{12} is an operation transforming S_1 into S_2: $\mathsf{S}_2 = g_{12}\mathsf{S}_1$.

The sectional layer group $\bar{\mathsf{F}}_{12}$ of the central plane with normal $\mathbf{n}$ and at a position $s\mathbf{d}$ under the action of the space group $\mathcal{F}_{12}$ is generally expressed as

$$\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}, \qquad (5.2.5.4)$$

where the halving subgroup $\widehat{\mathsf{F}}_{12}$ is the floating sectional layer group at a general position $s\mathbf{d}$. The operation $\underline{s}_{12}$ inverts the normal $\mathbf{n}$ and thus exchanges half-spaces on the left and right sides of the wall, where the left side is occupied by the state S_1 and the right side by the state S_2 in the initial twin. *These operations appear only at special positions of the central plane*. Since the half-spaces are occupied by domain states S_1 and S_2, their exchange is accompanied by an exchange of domain states on both sides of the wall. The operation $\underline{s}_{12}$ changes neither S_1 nor S_2 and hence it results in a *reversed domain twin* which has domain state S_2 on the left side and the domain state S_1 on the right side of the wall.

The *unordered domain pair* $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$ has the symmetry described by the group

$$\mathcal{J}_{12} = \mathcal{F}_{12} \cup j_{12}^*\mathcal{F}_{12}, \qquad (5.2.5.5)$$

where j_{12}^* is an operation that exchanges S_1 and S_2, $j_{12}^*\mathsf{S}_1 = \mathsf{S}_2$, $j_{12}^*\mathsf{S}_2 = \mathsf{S}_1$. Since for an unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$, the symmetry operations of the left coset $j_{12}^*\mathcal{F}_{12}$ are also symmetry operations of the unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$. If such an operation j_{12}^* and hence the whole coset $j_{12}^*\mathcal{F}_{12}$ of state-reversing operations exists, then the domain pair is called *transposable*. Otherwise $\mathcal{J}_{12} = \mathcal{F}_{12}$ and the domain pair is called *non-transposable*.

The sectional layer group of the space group $\mathcal{J}_{12}$ can therefore be generally written in the form

$$\bar{\mathsf{J}}_{12} = \widehat{\mathsf{F}}_{12} \cup r_{12}^*\widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12} \cup \underline{t}_{12}^*\widehat{\mathsf{F}}_1. \qquad (5.2.5.6)$$

In the general case, the group $\bar{\mathsf{J}}_{12}$ contains three halving subgroups which intersect at the subgroup $\widehat{\mathsf{F}}_{12}$ of index four: the subgroup $\widehat{\mathsf{J}}_{12} = \widehat{\mathsf{F}}_{12} \cup r_{12}^*\widehat{\mathsf{F}}_{12}$ is the floating subgroup of $\bar{\mathsf{J}}_{12}$; the coset $r_{12}^*\widehat{\mathsf{F}}_{12}$ is present if and only if the domain pair is transposable. The group $\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}$ is the sectional layer group for the ordered domain pair defined above. Finally, the group $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}_{12}^*\widehat{\mathsf{F}}_{12}$ is the symmetry group of the twin [see (5.2.5.2)]. Notice that it is itself not a sectional layer group of the space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ involved unless $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12}$, which occurs in the case of a non-transposable domain pair and of a general position of the central plane.

Since the cosets can be set-theoretically expressed as differences of groups: $r_{12}^*\widehat{\mathsf{F}}_{12} = \widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}$ and $\underline{s}_{12}\widehat{\mathsf{F}}_{12} = \bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12}$,

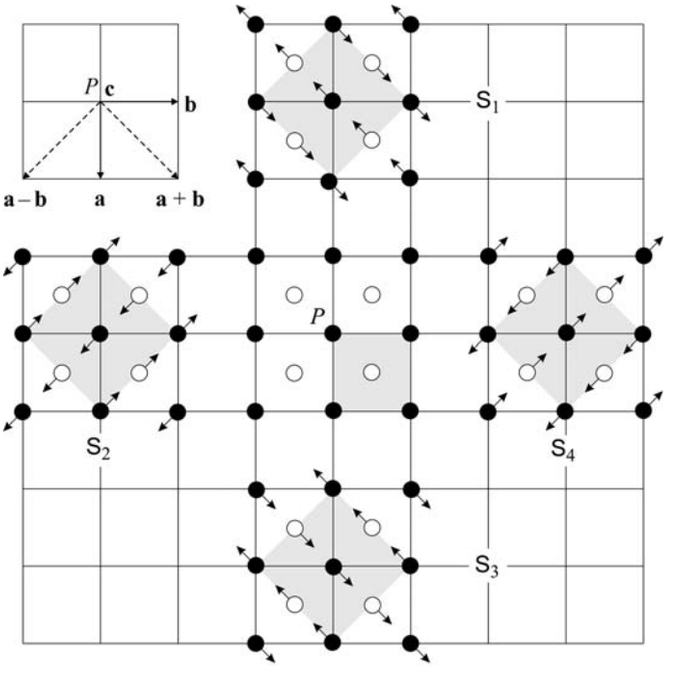

Fig. 5.2.5.5. The unit cell of the parent structure of calomel and the cells of four ferroic domain states.

while $\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [r_{12}^*\widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}]$, we receive a compact set-theoretical expression for the symmetry group of the twin in terms of four sectional layer groups:

$$\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [(\widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}) \cup (\bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12})]. \qquad (5.2.5.7)$$

Thus the symmetry group T_{12} of the twin can be expressed in terms of two sectional layer groups $\bar{\mathsf{F}}_{12}$, $\bar{\mathsf{J}}_{12}$ and their floating subgroups $\widehat{\mathsf{F}}_{12}$, $\widehat{\mathsf{J}}_{12}$, respectively. These four sectional layer groups can be found in the scanning tables.

As an illustrative example, we consider below a domain twin with a ferroelastic wall in the orthorhombic ferroelastic phase of the calomel crystal Hg_2Cl_2. Original analysis which includes the domain twin with antiphase boundary is given by Janovec & Zikmund (1993). Another analysis performed prior to the scanning tables is that of the domain twin in the KSCN crystal (Janovec *et al.*, 1989). Various cases of domain twins in fullerene C_{60} have also been analysed with the use of scanning tables (Janovec & Kopský, 1997; Saint-Grégoire *et al.*, 1997).

Example

The parent phase of calomel has a tetragonal body-centred structure of space-group symmetry $I4/mmm$ (D_{4h}^{17}), where lattice points are occupied by calomel molecules which have the form of Cl–Hg–Hg–Cl chains along the c axis. The crystallographic coordinate system is defined by vectors of the conventional tetragonal basis $\mathbf{a}_t = a\mathbf{e}_x$, $\mathbf{b}_t = a\mathbf{e}_y$, $\mathbf{c}_t = c\mathbf{e}_z$ with reference to the Cartesian basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ and the origin P is chosen at the centre of gravity of one of the calomel molecules. The parent structure projected onto the $z = 0$ plane is depicted in the middle of Fig. 5.2.5.5, where full and empty circles denote the centres of gravity at the levels $z = 0$ and $z = c/2$, respectively.

The ferroic phase is orthorhombic with a space-group symmetry of the type $Cmcm$ (D_{2h}^{17}), the conventional orthorhombic cell is based on vectors $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$ and contains two original cells. The conventional cell of the original tetragonal structure S and the cells of the four single

Table 5.2.5.1. *Symmetries of domain states and domain pairs in a calomel crystal*

All groups in this table are expressed by their Hermann–Mauguin symbols with reference to orthorhombic basis $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$.

Object	Symmetry group	Type
Parent phase	$\mathcal{G} = I4/mmm$	D_{4h}^{17}
S_1	$\mathcal{F}_1 = Am_{x\bar{y}}a_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
S_2	$\mathcal{F}_2 = Bb_{x\bar{y}}m_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
$(\mathsf{S}_1, \mathsf{S}_2)$	$\mathcal{F}_{12} = Pn_{x\bar{y}}n_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{12}
$\{\mathsf{S}_1, \mathsf{S}_2\}$	$\mathcal{J}_{12} = P4_{2z}^*/m_z n_{xy} m_x^*$ ($\mathbf{b}_t/2$)	D_{4h}^{14} $[D_{2h}^{12}]$

domain states S_1, S_2, S_3 and S_4 are shaded in Fig. 5.2.5.5. The arrows represent spontaneous shifts (x, x), $(-x, x)$, $(-x, -x)$ and $(x, -x)$ of gravity centres of molecules. The two single domain states S_1 and S_3 have the symmetry *Amam* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$); the other two single domain states S_2 and S_4 have the symmetry *Bbmm* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$), where the Hermann–Mauguin symbols refer to the orthorhombic basis. There are two classes of domain pairs, represented by the pairs $\{\mathsf{S}_1, \mathsf{S}_2\}$ and $\{\mathsf{S}_1, \mathsf{S}_3\}$, which result in domain walls referred to as a ferroelastic domain wall and an antiphase boundary, respectively. We shall consider the first of these cases.

The two single domain states S_1, S_2 and the unordered pair $\{\mathsf{S}_1, \mathsf{S}_2\}$ are represented in Fig. 5.2.5.6. The symmetries of the single domain states and of both the ordered and unordered pair are given in Table 5.2.5.1, where subscripts indicate the orientation of symmetry elements with reference to the Cartesian basis and an asterisk denotes operations that exchange the single domain states.

We consider the domain walls of the orientation (100) with reference to the original tetragonal basis ($\mathbf{a}_t$, $\mathbf{b}_t$, $\mathbf{c}_t$). This is the orientation with the Miller indices (110) with reference to the orthorhombic basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$). Consulting the scanning table No. 136 for the group $\mathcal{J}_{12} = P4_{2z}^*/m_z n_{xy} m_x^*$ ($\mathbf{b}_t/2$), we find the scanning group $Bm_y m_z m_x$ ($\mathbf{b}_t/2$) with reference to its conventional basis ($\mathbf{a}' = 2\mathbf{b}_t$, $\mathbf{b}' = \mathbf{c}_t$, $\mathbf{d} = 2\mathbf{a}_t$), where $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$. Applying the results of the scanning table with the shift by $\mathbf{b}_t/2 = \mathbf{a}'/4$, we obtain the sectional layer groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathsf{J}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). Analogously, for the space group $\mathcal{F}_{12}$, we obtain the sectional layer groups $\bar{\mathsf{F}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). All these groups are collected in the Table 5.2.5.2 in two notations. In this table, with a specified basis, each standard symbol contains the same information as the optional symbol. Optional symbols contain subscripts which explicitly specify the orientations of symmetry elements with reference to the Cartesian coordinate system ($\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$), asterisks and underlines have the meaning specified above. The lattice symbol p means the common lattice $T(2\mathbf{b}_t, \mathbf{c}_t) = T(\mathbf{a}', \mathbf{b}')$ of all sectional layer groups and twin symmetries. The Hermann–Mauguin symbols are written with reference to the coordinate systems ($P + s\mathbf{d}$; $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$).

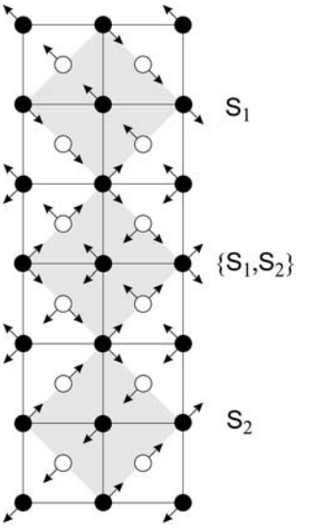

Fig. 5.2.5.6. The unordered domain pair between the two domain states.

The twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$ is determined by the relation (5.2.5.7). This means, in practice, that we have to find the groups $\bar{\mathsf{J}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$, $\bar{\mathsf{F}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ from which we obtain the group $\mathsf{T}_{12}(s\mathbf{d})$. If tables of subgroups of layer groups were available, it would be sufficient to look up the subgroups which lie between $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ and recognize the three groups $\bar{\mathsf{F}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$ and $\mathsf{T}_{12}(s\mathbf{d})$.

Optional symbols facilitate this determination considerably. To get the twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$, we look up the optional symbol for the group $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and eliminate elements that are either only underlined or that are only labelled by an asterisk. Or, *vice versa*, we leave only those elements that are not labelled at all or that are at the same time underlined and labelled by an asterisk. The resulting twin symmetries are given in the lower part of Table 5.2.5.2.

The implications of this symmetry analysis on the structure of domain walls at $0\mathbf{d}$ and $\frac{1}{4}\mathbf{d}$ are illustrated in Fig. 5.2.5.7. Shaded areas represent the domain states at infinity. The left-hand part of the figure corresponds to the location of the central plane at $0\mathbf{d}$, the right-hand part to the location at $\frac{1}{4}\mathbf{d}$. The twin

Table 5.2.5.2. *Sectional layer groups of space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ in the conventional basis ($\mathbf{a}' = 2\mathbf{b}_t$, $\mathbf{b}' = \mathbf{c}_t$, $\mathbf{d} = 2\mathbf{a}_t$) of the scanning group $Bm_y m_z m_x$ and the respective twin symmetries*

Space group	Plane (*hkl*)	Location	Sectional layer group		
		$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	Standard symbol	Optional symbol
$\mathcal{F}_{12}$	(110)	$0\mathbf{d}$	$\bar{\mathsf{F}}_{12}(0\mathbf{d})$	$p12/m1$ ($\mathbf{b}_t/2$)	$p1\underline{2}_z/m_z1$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$	$p12/m1$	$p1\underline{2}_z/m_z1$
		$s\mathbf{d}$	$\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}$	$p1m1$	$p1m_z1$
$\mathcal{J}_{12}$		$0\mathbf{d}$	$\bar{\mathsf{J}}_{12}(0\mathbf{d})$	$pmmm$ ($\mathbf{b}_t/2$)	$p2_y^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{m}_x^*$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$	$pmma$	$p\underline{2}_{1y}^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{a}_x^*$
		$s\mathbf{d}$	$\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathcal{J}}_{12}$	$pmm2$	$pm_y^*m_z2_x^*$
Twin symmetries		Location	$\mathsf{T}_{12}(s\mathbf{d})$	Symmetry of the twin	
		$0\mathbf{d}$	$\mathsf{T}_{12}(0\mathbf{d})$	$p2mm$	$p2_y^*m_z\underline{m}_x^*$
		$\frac{1}{4}\mathbf{d}$	$\mathsf{T}_{12}(\frac{1}{4}\mathbf{d})$	$p2_1ma$	$p\underline{2}_{1y}^*m_z\underline{a}_x^*$
		$s\mathbf{d}$	$\mathsf{T}_{12}(s\mathbf{d})$	$p1m1$	$p1m_z1$

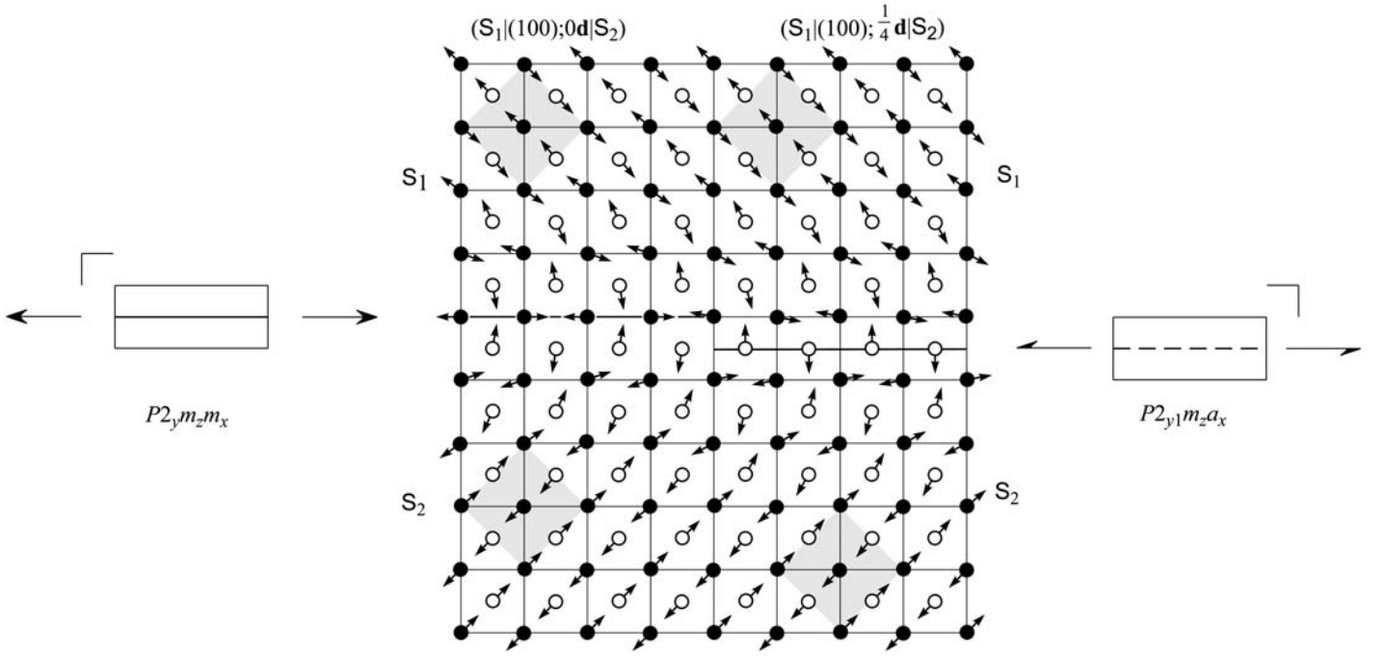

Fig. 5.2.5.7. The structures and symmetries of domain twins in calomel corresponding to two different special positions of the wall.

symmetries $\mathsf{T}_{12}(0\mathbf{d}) = p2_y m_z m_x$ and $\mathsf{T}_{12}(\frac{1}{4}\mathbf{d}) = p2_{1y} m_z a_x$ determine the relationship between the structures in the two half-spaces. The trivial symmetry operations form the layer group $p1m_z1$ in both cases and leave invariant the structures in both half-spaces. The nontrivial symmetry operations map the structure in one of the half-spaces onto the structure in the other half-space and back. The symmetry of the central plane is given by the groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ because the states S_1 and S_2 meet at this plane.

The arrows that represent the shift of calomel molecules in the xy plane may rotate and change their amplitude as we approach the central plane because the symmetry requirements are relaxed to those imposed by the layer group $p1m_z1$ consisting of trivial symmetry operations of the twin. The nontrivial twin symmetries determine the relationship between the structures in the two half-spaces, so that the rotation and change of amplitude in these two half-spaces are correlated. The symmetry of the central plane requires, in the left-hand part of the figure, that the arrows at black circles are aligned along the plane and that they are of the same lengths and alternating direction. The arrows at the empty circles in the right-hand part of the figure are nearly perpendicular to the plane, of the same lengths and of alternating direction in accordance with the central-plane symmetry. They are shown in the figure as strictly perpendicular to the plane; however, slight shifts of the atoms parallel to the plane can be expected because the arrows mean that the atoms are actually already out of the central plane.

Summary: In the analysis of domain twins, we know the structures of the two domain states, in our case the orientation of arrows, at infinity. In the example above, we considered two cases in both of which the layer group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ contains all four types of the twin operations – two types of symmetry operations and two types of twin-reversing operations. In this case, we summarize the results of the symmetry analysis as follows. (i) The floating layer group $\widehat{\mathsf{F}}_{12}$ determines the allowed changes of the structures on the path from infinity (physically this means the domain bulk) towards the central plane. (ii) Operations of the coset $\underline{t}^*_{12}\widehat{F}_{12}$ correlate the changes in the two half-spaces. (iii) The group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ as the symmetry of the central plane where the two half-spaces meet contains the twin symmetry $\mathsf{T}_{12}(s_o\mathbf{d})$ as its halving subgroup and therefore imposes additional conditions on the structure of the central plane in comparison with the conditions in its vicinity.

As always, the symmetry determines only the character of possible changes but neither their magnitude nor their dependence on the distance from the central plane. Thus, in the example considered, the symmetry arguments cannot predict the detailed dependence of the angle of rotation on the distance from the wall and they cannot predict whether and how the lengths of these arrows change.

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Laue class $C_i - \overline{1}$

Geometric class $C_1 - 1$

No. 1 $P1$ C_1^1

$$\mathcal{G} = P1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(hkl)	Any admissible choice	$P1$	$s\mathbf{d}$	$p1$	L01

Geometric class $C_i - \overline{1}$

No. 2 $P\overline{1}$ C_i^1

$$\mathcal{G} = P\overline{1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(hkl)	Any admissible choice	$P\overline{1}$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\overline{1}$	L02
			$[-s\mathbf{d}, s\mathbf{d}]$	$p1$	L01

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Laue class $C_i - \overline{1}$

Geometric class $C_1 - 1$

No. 1 $P1$ C_1^1

$$\mathcal{G} = P1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(hkl)	Any admissible choice	$P1$	$s\mathbf{d}$	$p1$	L01

Geometric class $C_i - \overline{1}$

No. 2 $P\overline{1}$ C_i^1

$$\mathcal{G} = P\overline{1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(hkl)	Any admissible choice	$P\overline{1}$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\overline{1}$	L02
			$[-s\mathbf{d}, s\mathbf{d}]$	$p1$	L01

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Laue class C_{2h} – $2/m$

Geometric class C_2 – 112

No. 3 $P2$ C_2^1

$\mathcal{G} = P121$ UNIQUE AXIS b

$\mathcal{G} = P112$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$ $\mathbf{a}$ $\mathbf{b}$	$P112$	$s\mathbf{d}$	$p112$	L03
UNIQUE AXIS c (001)	$\mathbf{a}$ $\mathbf{b}$ $\mathbf{c}$				
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$ $n\mathbf{c}-m\mathbf{a}$ $p\mathbf{c}+q\mathbf{a}$	$P211$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p211$	L08
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$ $n\mathbf{a}-m\mathbf{b}$ $p\mathbf{a}+q\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01

No. 4 $P2_1$ C_2^2

$\mathcal{G} = P12_11$ UNIQUE AXIS b

$\mathcal{G} = P112_1$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$ $\mathbf{a}$ $\mathbf{b}$	$P112_1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS c (001)	$\mathbf{a}$ $\mathbf{b}$ $\mathbf{c}$				
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$ $n\mathbf{c}-m\mathbf{a}$ $p\mathbf{c}+q\mathbf{a}$	$P2_111$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2_111$	L09
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$ $n\mathbf{a}-m\mathbf{b}$ $p\mathbf{a}+q\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01

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No. 5 $C2$ C_2^3

$\mathcal{G} = C121$ UNIQUE AXIS b

CELL CHOICE 1

$\mathcal{G} = A112$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$B211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd	$C211$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c211$	L10
		p odd			$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{p}1$	L01
		n odd		$I211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
		p odd			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 5 $C2$ C_2^3

$\mathcal{G} = A121$ UNIQUE AXIS b

CELL CHOICE 2

$\mathcal{G} = B112$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$C211$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c211$	L10
			q odd		$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{p}1$	L01
			m odd	$I211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
			q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
			m odd	$B211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 5 $C2$ C_2^3

$\mathcal{G} = I121$ UNIQUE AXIS b

CELL CHOICE 3

$\mathcal{G} = I112$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$I112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS c							
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$I211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
		or			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd				
		p odd	q even				
		p odd	q odd	$B211$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n odd	m odd	$C211$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c211$	L10
					$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{p}1$	L01

Geometric class C_s – 11m

No. 6 Pm C_s^1

$\mathcal{G} = P1m1$ UNIQUE AXIS b

$\mathcal{G} = P11m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P11m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p11m$	L04
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$Pm11$	$s\mathbf{d}$	$pm11$	L11
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				

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No. 7 Pc C_s^2

$\mathcal{G} = P1c1$ UNIQUE AXIS b

CELL CHOICE 1

$\mathcal{G} = P11a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P11a$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p11a$	L05
					$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b ($n0m$)	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c ($mn0$)	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Pb11$	$s\mathbf{d}$	$pb11$	L12
			q odd				
			m odd	$Pn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
			q odd				
			m odd	$Pc11$	$[s\mathbf{d}, (s+\frac{1}{2})\,\mathbf{d}]$	$p1$	L01
		p odd	q even				

No. 7 Pc C_s^2

$\mathcal{G} = P1n1$ UNIQUE AXIS b

CELL CHOICE 2

$\mathcal{G} = P11n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P11n$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p11n$	L05
					$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b ($n0m$)	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c ($mn0$)	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Pn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		p even	q odd				
		or					
		n even	m odd				
		p odd	q even				
		p odd	q odd	$Pc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n odd	m odd	$Pb11$	$s\mathbf{d}$	$pb11$	L12

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No. 7 *Pc* C_s^2

CELL CHOICE 3

$\mathcal{G} = P1a1$ UNIQUE AXIS *b*

$\mathcal{G} = P11b$ UNIQUE AXIS *c*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS *b* (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P11b$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p11b$	L05
UNIQUE AXIS *c* (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01
UNIQUE AXIS *b* $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS *c* $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$Pc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		p even	q odd				
		n even	m odd	$Pb11$	$s\mathbf{d}$	$pb11$	L12
		p odd					
		n odd		$Pn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		p odd					

No. 8 *Cm* C_s^3

CELL CHOICE 1

$\mathcal{G} = C1m1$ UNIQUE AXIS *b*

$\mathcal{G} = A11m$ UNIQUE AXIS *c*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS *b* (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A11m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
UNIQUE AXIS *c* (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS *b* $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS *c* $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$Bm11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
		p even	q odd				
		n even	m odd	$Cm11$	$s\mathbf{d}$	$cm11$	L13
		p odd					
		n odd		$Im11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
		p odd					

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No. 8 *Cm* C_s^3

CELL CHOICE 2

$\mathcal{G} = A1m1$ UNIQUE AXIS *b*

$\mathcal{G} = B11m$ UNIQUE AXIS *c*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS *b*							
(010)	**c**	**a**	**b**	$B11m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
UNIQUE AXIS *c*					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
(001)	**a**	**b**	**c**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS *b*							
$(n0m)$	**b**	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS *c*							
$(mn0)$	**c**	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$Cm11$	$s\mathbf{d}$	$cm11$	L13
			q odd				
			m odd	$Im11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
			q odd				
			m odd	$Bm11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
		p odd	q even				

No. 8 *Cm* C_s^3

CELL CHOICE 3

$\mathcal{G} = I1m1$ UNIQUE AXIS *b*

$\mathcal{G} = I11m$ UNIQUE AXIS *c*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS *b*							
(010)	**c**	**a**	**b**	$I11m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
UNIQUE AXIS *c*					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
(001)	**a**	**b**	**c**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS *b*							
$(n0m)$	**b**	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS *c*							
$(mn0)$	**c**	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$Im11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
		p even	q odd				
			or				
		n even	m odd				
		p odd	q even				
		p odd	q odd	$Bm11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
		n odd	m odd	$Cm11$	$s\mathbf{d}$	$cm11$	L13

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No. 9 Cc C_s^4

CELL CHOICE 1

$\mathcal{G} = C1c1$ UNIQUE AXIS b

$\mathcal{G} = A11a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A11a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11a$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Bb11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p even	q odd				
		n even	m odd	$Cc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q even				
		n even	m odd	$Cn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q odd				
		n odd	m odd	$Bn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p even	q odd				
		n odd	m odd	$Ic11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q even				
		n odd	m even	$Ib11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q odd				

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No. 9 Cc C_s^4

CELL CHOICE $\widetilde{1}$

$\mathcal{G} = A1a1$ UNIQUE AXIS b

$\mathcal{G} = B11b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B11b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11b$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$Cc11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p even	q odd				
		n even	m odd	$Bb11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q even				
		n even	m odd	$Ib11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q odd				
		n odd	m odd	$Ic11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p even	q odd				
		n odd	m odd	$Bn11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q even				
		n odd	m even	$Cn11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q odd				

No. 9 Cc C_s^4

CELL CHOICE 2

$\mathcal{G} = A1n1$ UNIQUE AXIS b

$\mathcal{G} = B11n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B11n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11n$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Cn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p even	q odd				
		n even	m odd	$Bn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q even				
		n even	m odd	$Ic11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q odd				
		n odd	m odd	$Ib11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p even	q odd				
		n odd	m odd	$Bb11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q even				
		n odd	m even	$Cc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q odd				

No. 9 Cc C_s^4

CELL CHOICE $\widetilde{2}$

$\mathcal{G} = C1n1$ UNIQUE AXIS b

$\mathcal{G} = A11n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A11n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11n$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$Bn11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p even	q odd				
		n even	m odd	$Cn11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q even				
		n even	m odd	$Cc11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q odd				
		n odd	m odd	$Bb11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p even	q odd				
		n odd	m odd	$Ib11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q even				
		n odd	m even	$Ic11$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q odd				

No. 9 Cc C_s^4

CELL CHOICE 3

$\mathcal{G} = I1a1$ UNIQUE AXIS b

$\mathcal{G} = I11b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$I11b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11b$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Ic11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p even	q odd				
		n even	m odd	$Ib11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q even				
		n even	m odd	$Bb11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q odd				
		n odd	m odd	$Cc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p even	q odd				
		n odd	m odd	$Cn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q even				
		n odd	m even	$Bn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q odd				

No. 9 Cc C_s^4

CELL CHOICE $\widetilde{3}$

$\mathcal{G} = I1c1$ UNIQUE AXIS b

$\mathcal{G} = I11a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$I11a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11a$	L05
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$Ib11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p even	q odd				
		n even	m odd	$Ic11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q even				
		n even	m odd	$Bn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		p odd	q odd				
		n odd	m odd	$Cn11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p even	q odd				
		n odd	m odd	$Cc11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		p odd	q even				
		n odd	m even	$Bb11$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		p odd	q odd				

Geometric class C_{2h} – 112/m

No. 10 $P2/m$ C_{2h}^1

$\mathcal{G} = P12/m1$ UNIQUE AXIS b

$\mathcal{G} = P112/m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p112/m$	L06
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$P2/m11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2/m11$	L14
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$	L11
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				

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No. 11 $P2_1/m$ C_{2h}^2

$\mathcal{G} = P12_1/m1$ UNIQUE AXIS b

$\mathcal{G} = P112_1/m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112_1/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11m$	L04
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$P2_1/m11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2_1/m11$	L15
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				

No. 12 $C2/m$ C_{2h}^3

$\mathcal{G} = C12/m1$ UNIQUE AXIS b

CELL CHOICE 1

$\mathcal{G} = A112/m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $(\mathbf{b}/4)$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$B2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $(\mathbf{a}'/4)$	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
		n even	m odd	$C2/m11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c2/m11$	L18
		p odd			$[s\mathbf{d}, -s\mathbf{d}]$	$cm11$	L13
		n odd		$I2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
		p odd			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

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No. 12 $C2/m$ C_{2h}^3

$\mathcal{G} = A12/m1$ UNIQUE AXIS b

CELL CHOICE 2

$\mathcal{G} = B112/m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $(\mathbf{a}/4)$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$C2/m11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c2/m11$	L18
			q odd		$[s\mathbf{d}, -s\mathbf{d}]$	$cm11$	L13
			m odd	$I2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
			q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $[(\mathbf{a}' + \mathbf{b}')/4]$	L15
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
			m odd	$B2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $(\mathbf{a}'/4)$	L15
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 12 $C2/m$ C_{2h}^3

$\mathcal{G} = I12/m1$ UNIQUE AXIS b

CELL CHOICE 3

$\mathcal{G} = I112/m$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$I112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $[(\mathbf{a} + \mathbf{b})/4]$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$I2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $[(\mathbf{a}' + \mathbf{b}')/4]$	L15
		or			$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
		n even	m odd				
		p odd	q even				
		p odd	q odd	$B2/m11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $(\mathbf{a}'/4)$	L15
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
		n odd	m odd	$C2/m11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c2/m11$	L18
					$[s\mathbf{d}, -s\mathbf{d}]$	$cm11$	L13

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 13, pp. 437–438.

No. 13 $P2/c$ C_{2h}^4

CELL CHOICE 1

$\mathcal{G} = P12/c1$ UNIQUE AXIS b

$\mathcal{G} = P112/a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/a$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p112/a$	L07
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{a}/4)$	L03
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$P2/b11$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2/b11$	L16
			q odd		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
			m odd	$P2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
			q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$ $(\mathbf{b}'/4)$	L08
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
			m odd	$P2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 13 $P2/c$ C_{2h}^4

CELL CHOICE 2

$\mathcal{G} = P12/n1$ UNIQUE AXIS b

$\mathcal{G} = P112/n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/n$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p112/n$	L07
UNIQUE AXIS c					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $[(\mathbf{a}+\mathbf{b})/4]$	L03
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$				
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$P2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$ $(\mathbf{b}'/4)$	L08
		or			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd				
		p odd	q even				
		p odd	q odd	$P2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n odd	m odd	$P2/b11$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2/b11$	L16
					$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12

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International Tables for Crystallography (2010). Vol. E, Scanning table for space group 14, pp. 438–439.

No. 13 $P2/c$ C_{2h}^4

$\mathcal{G} = P12/a1$ UNIQUE AXIS b

CELL CHOICE 3

$\mathcal{G} = P112/b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/b$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p112/b$	L07
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{b}/4)$	L03
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$P2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd	$P2/b11$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2/b11$	L16
		p odd			$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
		n odd		$P2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p odd			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$ $(\mathbf{b}'/4)$	L08
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 14 $P2_1/c$ C_{2h}^5

$\mathcal{G} = P12_1/c1$ UNIQUE AXIS b

CELL CHOICE 1

$\mathcal{G} = P112_1/a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112_1/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b $(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c $(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$P2_1/b11$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2_1/b11$	L17
			q odd		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
			m odd	$P2_1/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
			q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
			m odd	$P2_1/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 14 $P2_1/c$ C_{2h}^5

CELL CHOICE 2

$\mathcal{G} = P12_1/n1$ UNIQUE AXIS b

$\mathcal{G} = P112_1/n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112_1/n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
($n0m$)	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
($mn0$)	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$P2_1/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ ($\mathbf{b}'/4$)	L09
		or			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd				
		p odd	q even				
		p odd	q odd	$P2_1/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n odd	m odd	$P2_1/b11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2_1/b11$	L17
					$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$ ($\mathbf{a}'/4$)	L12

No. 14 $P2_1/c$ C_{2h}^5

CELL CHOICE 3

$\mathcal{G} = P12_1/a1$ UNIQUE AXIS b

$\mathcal{G} = P112_1/b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112_1/b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
UNIQUE AXIS b							
($n0m$)	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
($mn0$)	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd		$P2_1/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd	$P2_1/b11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2_1/b11$	L17
		p odd			$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$ ($\mathbf{a}'/4$)	L12
		n odd		$P2_1/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{1}$	L02
		p odd			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ ($\mathbf{b}'/4$)	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 15, pp. 440–445.

No. 15 $C2/c$ C_{2h}^6

CELL CHOICE 1

$\mathcal{G} = C12/c1$ UNIQUE AXIS b

$\mathcal{G} = A112/a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	**c**	**a**	**b**	$A112/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $(\mathbf{b}/4)$	L07
(001)	**a**	**b**	**c**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}/4)$	L03
UNIQUE AXIS b							
$(n0m)$	**b**	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	**c**	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$B2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $(\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n even	m odd	$C2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L12
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n even	m odd	$C2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$ $(\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m odd	$B2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $(\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n odd	m odd	$I2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n odd	m even	$I2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12

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No. 15 $C2/c$ C_{2h}^6

CELL CHOICE $\widetilde{1}$

$\mathcal{G} = A12/a1$ UNIQUE AXIS b

$\mathcal{G} = B112/b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B112/b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/b$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $(\mathbf{a}/4)$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}/4)$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$C2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\overline{1}}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n even	m odd	$B2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $(\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n even	m odd	$I2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m odd	$I2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n odd	m odd	$B2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $(\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n odd	m even	$C2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\overline{1}}$	L02
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$ $(\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01

No. 15 $C2/c$ C_{2h}^6

$\mathcal{G} = A12/n1$ UNIQUE AXIS b

CELL CHOICE 2

$\mathcal{G} = B112/n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$B112/n$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p112/b\ (\mathbf{a}/4)$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ [(\mathbf{a}+\mathbf{b})/4]$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$C2/n11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$c211\ (\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n even	m odd	$B2/n11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q even		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2/b11\ (\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11\ (\mathbf{a}'/4)$	L12
		n even	m odd	$I2/c11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q odd		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2/b11\ [(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11\ (\mathbf{a}'/4)$	L12
		n odd	m odd	$I2/b11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p even	q odd		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2_1/b11\ [(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m odd	$B2/b11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q even		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2_1/b11\ (\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m even	$C2/c11$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q odd		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$c211$	L10
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01

No. 15 $C2/c$ C_{2h}^6

CELL CHOICE $\widetilde{2}$

$\mathcal{G} = C12/n1$ UNIQUE AXIS b

$\mathcal{G} = A112/n$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$A112/n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $(\mathbf{b}/4)$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}+\mathbf{b})/4]$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$B2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $(\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n even	m odd	$C2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$ $(\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n even	m odd	$C2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m odd	$B2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $(\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m odd	$I2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m even	$I2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

No. 15 $C2/c$ C_{2h}^6

CELL CHOICE 3

$\mathcal{G} = I12/a1$ UNIQUE AXIS b

$\mathcal{G} = I112/b$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$I112/b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/b$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $[(\mathbf{a}+\mathbf{b})/4]$	L07
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}/4)$	L03
UNIQUE AXIS b							
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$I2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n even	m odd	$I2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n even	m odd	$B2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $(\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n odd	m odd	$C2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m odd	$C2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$ $(\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m even	$B2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $(\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

No. 15 $C2/c$ C_{2h}^6

CELL CHOICE $\widetilde{3}$

$\mathcal{G} = I12/c1$ UNIQUE AXIS b

$\mathcal{G} = I112/a$ UNIQUE AXIS c

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b							
(010)	**c**	**a**	**b**	$I112/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
UNIQUE AXIS c					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $[(\mathbf{a}+\mathbf{b})/4]$	L07
(001)	**a**	**b**	**c**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}/4)$	L03
UNIQUE AXIS b							
$(n0m)$	**b**	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$				
UNIQUE AXIS c							
$(mn0)$	**c**	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$				
		n odd	m even	$I2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
		n even	m odd	$I2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n even	m odd	$B2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2/b11$ $(\mathbf{a}'/4)$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
		n odd	m odd	$C2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$ $(\mathbf{b}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m odd	$C2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p\bar{1}}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
		n odd	m even	$B2/b11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
		p odd	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $(\mathbf{a}'/4)$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12

Laue class D_{2h} – *mmm*

Geometric class D_2 – 222

No. 16 $P222$ D_2^1

$$\mathcal{G} = P222$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P222$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p222$	L19
(100)	**b**	**c**	**a**		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**				

No. 17 $P222_1$ D_2^2

$$\mathcal{G} = P222_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P222_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p121$	L08
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(100)	**b**	**c**	**a**	$P22_12$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p22_12$	L20
					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**	$P2_122$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2_122$ $(\mathbf{a}'/4)$	L20
					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03

No. 18 $P2_12_12$ D_2^3

$$\mathcal{G} = P2_12_12$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P2_12_12$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p2_12_12$	L21
					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$P2_122_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**	$P22_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 19 $P2_12_12_1$ D_2^4

$$\mathcal{G} = P2_12_12_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_111$ ($\mathbf{b}'/4$)	L09
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
(100)	**b**	**c**	**a**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**				

No. 20 $C222_1$ D_2^5

$$\mathcal{G} = C222_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$C222_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c211$	L10
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
(100)	**b**	**c**	**a**	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**	$A2_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/4$)	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ ($\mathbf{a}'/4$)	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/4$)	L03

No. 21 $C222$ D_2^6

$$\mathcal{G} = C222$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$C222$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$c222$	L22
					$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{p}112$	L03
(100)	**b**	**c**	**a**	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 22 $F222$ D_2^7

$$\mathcal{G} = F222$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ $[(\mathbf{a}' + \mathbf{b}')/4]$	L22
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03

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No. 23 $I222$ D_2^8

$$\mathcal{G} = I222$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 24 $I2_12_12_1$ D_2^9

$$\mathcal{G} = I2_12_12_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{b}'/4)$	L20
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/4)$	L20
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

Geometric class C_{2v} – *mm2*

No. 25 $Pmm2$ C_{2v}^1

$$\mathcal{G} = Pmm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Pmm2$	$s\mathbf{d}$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Pm2m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pm2m$	L27
					$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$	L11
(010)	**c**	**a**	**b**	$P2mm$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2mm$	L27
					$[s\mathbf{d}, -s\mathbf{d}]$	$p1m1$	L11

No. 26 $Pmc2_1$ C_{2v}^2

$$\mathcal{G} = Pmc2_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Pmc2_1$	$[s\mathbf{d}, (s + \frac{1}{2})\mathbf{d}]$	$pm11$	L11
(100)	**b**	**c**	**a**	$Pb2_1m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pb2_1m$	L29
					$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
(010)	**c**	**a**	**b**	$P2_1ma$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2_1ma$	L28
					$[s\mathbf{d}, -s\mathbf{d}]$	$p1m1$	L11

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No. 27 *Pcc*2 C_{2v}^3

$$\mathcal{G} = Pcc2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pcc*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*p*112	L03
(100)	**b**	**c**	**a**	*Pb*2*b*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pb*2*b*	L30
					$[s\mathbf{d}, -s\mathbf{d}]$	*pb*11	L12
(010)	**c**	**a**	**b**	*P*2*aa*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*p*2*aa*	L30
					$[s\mathbf{d}, -s\mathbf{d}]$	*p*1*a*1	L12

No. 28 *Pma*2 C_{2v}^4

$$\mathcal{G} = Pma2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pma*2	$s\mathbf{d}$	*pma*2	L24
(100)	**b**	**c**	**a**	*Pc*2*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*121	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*11*m*	L04
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01
(010)	**c**	**a**	**b**	*P*2*mb*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*p*2*mb*	L31
					$[s\mathbf{d}, -s\mathbf{d}]$	*p*1*m*1 $(\mathbf{b}'/4)$	L11

No. 29 *Pca*2_1 C_{2v}^5

$$\mathcal{G} = Pca2_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pca*2_1	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*p*1*a*1	L12
(100)	**b**	**c**	**a**	*Pc*2_1*b*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*12$_1$1	L09
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*11*b*	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01
(010)	**c**	**a**	**b**	*P*2_1*ab*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*p*2_1*ab*	L33
					$[s\mathbf{d}, -s\mathbf{d}]$	*p*1*a*1 $(\mathbf{b}'/4)$	L12

No. 30 *Pnc*2 C_{2v}^6

$$\mathcal{G} = Pnc2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnc*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*p*112	L03
(100)	**b**	**c**	**a**	*Pb*2*n*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pb*2*n*	L34
					$[s\mathbf{d}, -s\mathbf{d}]$	*pb*11 $(\mathbf{a}'/4)$	L12
(010)	**c**	**a**	**b**	*P*2*na*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*211	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*11*a*	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01

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No. 31 $Pmn2_1$ C_{2v}^7

$$\mathcal{G} = Pmn2_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Pmn2_1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(100)	**b**	**c**	**a**	$Pn2_1m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**	$P2_1mn$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2_1mn$	L32
					$[s\mathbf{d}, -s\mathbf{d}]$	$p1m1$	L11

No. 32 $Pba2$ C_{2v}^8

$$\mathcal{G} = Pba2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Pba2$	$s\mathbf{d}$	$pba2$	L25
(100)	**b**	**c**	**a**	$Pc2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**	$P2cb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 33 $Pna2_1$ C_{2v}^9

$$\mathcal{G} = Pna2_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Pna2_1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1a1$ $(\mathbf{b}/4)$	L12
(100)	**b**	**c**	**a**	$Pc2_1n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_11$	L09
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**	$P2_1nb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_111$	L09
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 34 *Pnn*2 C_{2v}^{10}

$$\mathcal{G} = Pnn2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnn*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*p*112	L03
(100)	**b**	**c**	**a**	*Pn*2*n*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*121	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*11*n*	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01
(010)	**c**	**a**	**b**	*P*2*nn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*211	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*11*n*	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01

No. 35 *Cmm*2 C_{2v}^{11}

$$\mathcal{G} = Cmm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmm*2	$s\mathbf{d}$	*cmm*2	L26
(100)	**b**	**c**	**a**	*Bm*2*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pm*2*m*	L27
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pm*2*a* ($\mathbf{a}'/4$)	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pm*11	L11
(010)	**c**	**a**	**b**	*A*2*mm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*mm*	L27
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2*mb* ($\mathbf{b}'/4$)	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*m*1	L11

No. 36 *Cmc*2_1 C_{2v}^{12}

$$\mathcal{G} = Cmc2_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmc*2_1	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*cm*11	L13
(100)	**b**	**c**	**a**	*Bb*2_1*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pb*2_1*m*	L29
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pb*2_1*a* ($\mathbf{a}'/4$)	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11	L12
(010)	**c**	**a**	**b**	*A*2_1*ma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2_1*ma*	L28
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2_1*mn*	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*m*1	L11

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No. 37 *Ccc*2 C_{2v}^{13}

$$\mathcal{G} = Ccc2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ccc*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03
(100)	**b**	**c**	**a**	*Bb*2*b*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pb*2*b*	L30
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pb*2*n* ($\mathbf{a}'/4$)	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11	L12
(010)	**c**	**a**	**b**	*A*2*aa*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*aa*	L30
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2*an* ($\mathbf{b}'/4$)	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*a*1	L12

No. 38 *Amm*2 C_{2v}^{14}

$$\mathcal{G} = Amm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Amm*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*pmm*2	L23
(100)	**b**	**c**	**a**	*Cm*2*m*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*cm*2*m*	L35
					$[s\mathbf{d}, -s\mathbf{d}]$	*cm*11	L13
(010)	**c**	**a**	**b**	*B*2*mm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*mm*	L27
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2$_1$*ma*	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*m*1	L11

No. 39* *Aem*2 C_{2v}^{15}

$$\mathcal{G} = Abm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Abm*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*pbm*2	L24
(100)	**b**	**c**	**a**	*Cm*2*a*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*cm*2*e*	L36
					$[s\mathbf{d}, -s\mathbf{d}]$	*cm*11 ($\mathbf{a}'/4$)	L13
(010)	**c**	**a**	**b**	*B*2*cm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*aa*	L30
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2$_1$*am*	L29
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*a*1	L12

*New symbol. Old symbol: *Abm*2.

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No. 40 *Ama*2 C_{2v}^{16}

$$\mathcal{G} = Ama2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ama*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*pma*2	L24
(100)	**b**	**c**	**a**	*Cc*2*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*c*121	L10
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}11m$	L04
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1	L01
(010)	**c**	**a**	**b**	*B*2*mb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*mb*	L31
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$ ($\mathbf{b}'/4$)	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$ ($\mathbf{b}'/4$)	L11

No. 41* *Aea*2 C_{2v}^{17}

$$\mathcal{G} = Aba2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Aba*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*pba*2	L25
(100)	**b**	**c**	**a**	*Cc*2*a*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*c*211	L10
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}11n$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}1$	L01
(010)	**c**	**a**	**b**	*B*2*cb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*an*	L34
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ab$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$ ($\mathbf{b}'/4$)	L12

*New symbol. Old symbol: *Aba*2.

No. 42 *Fmm*2 C_{2v}^{18}

$$\mathcal{G} = Fmm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Fmm*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*cmm*2	L26
(100)	**b**	**c**	**a**	*Fm*2*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*cm*2*m*	L35
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*cm*2*e* ($\mathbf{a}'/4$)	L36
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*cm*11	L13
(010)	**c**	**a**	**b**	*F*2*mm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*c*2*mm*	L35
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*c*2*me* ($\mathbf{b}'/4$)	L36
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*c*1*m*1	L13

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No. 43 $Fdd2$ C_{2v}^{19}

$$\mathcal{G} = Fdd2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Fdd2$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$	L03
(100)	**b**	**c**	**a**	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}, \frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$	L10
						$c121$ $(\mathbf{a}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}, \frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11b$	L09
						$\widehat{p}11a$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01
(010)	**c**	**a**	**b**	$F2dd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}, \frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c211$	L10
						$c211$ $(\mathbf{b}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}, \frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11b$	L09
						$\widehat{p}11a$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01

No. 44 $Imm2$ C_{2v}^{20}

$$\mathcal{G} = Imm2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Imm2$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Im2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(010)	**c**	**a**	**b**	$I2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11

No. 45 $Iba2$ C_{2v}^{21}

$$\mathcal{G} = Iba2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$Iba2$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(100)	**b**	**c**	**a**	$Ic2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$ $(\mathbf{a}'/4)$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(010)	**c**	**a**	**b**	$I2cb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2aa$	L30
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ab$ $(\mathbf{b}'/4)$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12

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No. 46 *Ima*2 C_{2v}^{22}

$$\mathcal{G} = Ima2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ima*2	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	*pma*2	L24
(100)	**b**	**c**	**a**	*Ic*2*m*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pb*2*n*	L34
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1m$ $(\mathbf{a}'/4)$	L29
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11 $(\mathbf{a}'/4)$	L12
(010)	**c**	**a**	**b**	*I*2*mb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*2*mb*	L31
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ma$ $(\mathbf{b}'/4)$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*m*1 $(\mathbf{b}'/4)$	L11

Geometric class D_{2h} – *mmm*

No. 47 *Pmmm* D_{2h}^{1}

$$\mathcal{G} = P\frac{2}{m}\frac{2}{m}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pmmm*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*pmmm*	L37
(100)	**b**	**c**	**a**		$[s\mathbf{d}, -s\mathbf{d}]$	*pmm*2	L23
(010)	**c**	**a**	**b**				

No. 48 *Pnnn* D_{2h}^{2}

$$\mathcal{G} = P\frac{2}{n}\frac{2}{n}\frac{2}{n} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnnn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*p*222	L19
(100)	**b**	**c**	**a**	$(\boldsymbol{\tau}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L07
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*112	L03

$\boldsymbol{\tau} = \mathbf{a}' + \mathbf{b}' + \mathbf{d}$.

No. 48 *Pnnn* D_{2h}^{2}

$$\mathcal{G} = P\frac{2}{n}\frac{2}{n}\frac{2}{n} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnnn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*222 $[(\mathbf{a}'+\mathbf{b}')/4]$	L19
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*112 $[(\mathbf{a}'+\mathbf{b}')/4]$	L03

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No. 49 *Pccm* D_{2h}^3

$$\mathcal{G} = P\frac{2}{c}\frac{2}{c}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pccm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	*Pbmb*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*pbmb*	L38
					$[s\mathbf{d}, -s\mathbf{d}]$	*pbm*2 $(\mathbf{b}'/4)$	L24
(010)	**c**	**a**	**b**	*Pmaa*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*pmaa*	L38
					$[s\mathbf{d}, -s\mathbf{d}]$	*pma*2 $(\mathbf{a}'/4)$	L24

No. 50 *Pban* D_{2h}^4

$$\mathcal{G} = P\frac{2}{b}\frac{2}{a}\frac{2}{n} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pban* $[(\mathbf{a}+\mathbf{b})/4]$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*pban* $[(\mathbf{a}+\mathbf{b})/4]$	L39
					$[s\mathbf{d}, -s\mathbf{d}]$	*pba*2	L25
(100)	**b**	**c**	**a**	*Pcna* $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $(\mathbf{a}'/4)$	L07
					$[\pm s\mathbf{d}\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**	*Pncb* $[(\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $(\mathbf{b}'/4)$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 50 *Pban* D_{2h}^4

$$\mathcal{G} = P\frac{2}{b}\frac{2}{a}\frac{2}{n} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pban*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	*pban*	L39
					$[s\mathbf{d}, -s\mathbf{d}]$	*pba*2 $[(\mathbf{a}+\mathbf{b})/4]$	L25
(100)	**b**	**c**	**a**	*Pcna*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $(\mathbf{a}'/4)$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
(010)	**c**	**a**	**b**	*Pncb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/b$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $(\mathbf{b}'/4)$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

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No. 51 *Pmma* D_{2h}^5

$$\mathcal{G} = P\frac{2}{m}\frac{2}{m}\frac{2}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pmma*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pmma*	L41
					$[s\mathbf{d}, -s\mathbf{d}]$	*pmm*2 (**a**/4)	L23
(100)	**b**	**c**	**a**	*Pmcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pm*2*m*	L27
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pm*11	L11
(010)	**c**	**a**	**b**	*Pbmm*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pbmm*	L40
					$[s\mathbf{d}, -s\mathbf{d}]$	*pbm*2	L24

No. 52 *Pnna* D_{2h}^6

$$\mathcal{G} = P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnna*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ (**a**/4)	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ (**a**/4)	L03
(100)	**b**	**c**	**a**	*Pncn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ $[(\mathbf{a}' + \mathbf{b}')/4]$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}' + \mathbf{b}')/4]$	L03
(010)	**c**	**a**	**b**	*Pbnn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pb*2*n* ($\mathbf{a}'$/4)	L34
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pb*11	L12

No. 53 *Pmna* D_{2h}^7

$$\mathcal{G} = P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pmna*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pm*2*a* (**a**/4)	L31
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pm*11	L11
(100)	**b**	**c**	**a**	*Pncm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(010)	**c**	**a**	**b**	*Pbmn*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pbmn*	L42
					$[s\mathbf{d}, -s\mathbf{d}]$	*pbm*2 $[(\mathbf{a}' + \mathbf{b}')/4]$	L24

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No. 54 *Pcca* D_{2h}^{8}

$$\mathcal{G} = P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pcca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ $(\mathbf{a}/4)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}/4)$	L03
(100)	**b**	**c**	**a**	*Pbcb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(010)	**c**	**a**	**b**	*Pbaa*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pbaa$	L43
					$[s\mathbf{d}, -s\mathbf{d}]$	$pba2$ $(\mathbf{a}'/4)$	L25

No. 55 *Pbam* D_{2h}^{9}

$$\mathcal{G} = P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pbam*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pbam$	L44
					$[s\mathbf{d}, -s\mathbf{d}]$	$pba2$	L25
(100)	**b**	**c**	**a**	*Pcma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ma$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(010)	**c**	**a**	**b**	*Pmcb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1b$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 56 *Pccn* D_{2h}^{10}

$$\mathcal{G} = P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pccn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $[(\mathbf{a}+\mathbf{b})/4]$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}+\mathbf{b})/4]$	L03
(100)	**b**	**c**	**a**	*Pbnb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
(010)	**c**	**a**	**b**	*Pnaa*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_1/a1$	L17
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2aa$ $(\mathbf{b}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$ $(\mathbf{b}'/4)$	L12

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No. 57 *Pbcm* D_{2h}^{11}

$$\mathcal{G} = P\,\frac{2}{b}\,\frac{2_1}{c}\,\frac{2_1}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pbcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1m$	L29
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(100)	**b**	**c**	**a**	*Pbma*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pbma$	L45
					$[s\mathbf{d}, -s\mathbf{d}]$	$pbm2$ $(\mathbf{a}'/4)$	L24
(010)	**c**	**a**	**b**	*Pmca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/m11$	L15
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2a$	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11

No. 58 *Pnnm* D_{2h}^{12}

$$\mathcal{G} = P\,\frac{2_1}{n}\,\frac{2_1}{n}\,\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnnm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	*Pnmn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(010)	**c**	**a**	**b**	*Pmnn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/m11$	L14
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 59 *Pmmn* D_{2h}^{13}

$$\mathcal{G} = P\,\frac{2_1}{m}\,\frac{2_1}{m}\,\frac{2}{n} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pmmn*	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pmmn$ $[(\mathbf{a}+\mathbf{b})/4]$	L46
				$[(\mathbf{a}+\mathbf{b})/4]$	$[s\mathbf{d}, -s\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	*Pmnm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
				$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $(\mathbf{a}'/4)$	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(010)	**c**	**a**	**b**	*Pnmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
				$[(\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/m1$ $(\mathbf{b}'/4)$	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11

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No. 59 *Pmmn* D_{2h}^{13}

$$\mathcal{G} = P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pmmn*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*pmmn*	L46
					$[s\mathbf{d}, -s\mathbf{d}]$	*pmm*2 $[(\mathbf{a}+\mathbf{b})/4]$	L23
(100)	**b**	**c**	**a**	*Pmnm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/m11$	L15
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pm*2*m* $(\mathbf{a}'/4)$	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pm*11 $(\mathbf{a}'/4)$	L11
(010)	**c**	**a**	**b**	*Pnmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_1/m1$	L15
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*p*2*mm* $(\mathbf{b}'/4)$	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*1*m*1 $(\mathbf{b}'/4)$	L11

No. 60 *Pbcn* D_{2h}^{14}

$$\mathcal{G} = P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pbcn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pb*2*n*	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11 $(\mathbf{a}/4)$	L12
(100)	**b**	**c**	**a**	*Pbna*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2/b11$	L16
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$ $(\mathbf{a}'/4)$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11	L12
(010)	**c**	**a**	**b**	*Pnca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/4)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*p*112 $(\mathbf{a}'/4)$	L03

No. 61 *Pbca* D_{2h}^{15}

$$\mathcal{G} = P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pbca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$	L33
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pb*11 $(\mathbf{a}'/4)$	L12

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No. 62 *Pnma* D_{2h}^{16}

$$\mathcal{G} = P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Pnma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_1/m1$	L15
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ma$ $(\mathbf{b}/4)$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$ $(\mathbf{b}/4)$	L11
(100)	**b**	**c**	**a**	*Pmcn*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/m11$	L15
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$ $(\mathbf{a}'/4)$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11
(010)	**c**	**a**	**b**	*Pbnm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1m$ $(\mathbf{a}'/4)$	L29
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

No. 63 *Cmcm* D_{2h}^{17}

$$\mathcal{G} = C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c2/m11$	L18
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cm2m$	L35
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cm11$	L13
(100)	**b**	**c**	**a**	*Bbmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmm$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbma$ $(\mathbf{a}'/4)$	L45
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$	L24
(010)	**c**	**a**	**b**	*Amma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmma$	L41
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $(\mathbf{b}'/4)$	L46
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$ $(\mathbf{a}'/4)$	L23

No. 64* *Cmce* D_{2h}^{18}

$$\mathcal{G} = C\frac{2}{m}\frac{2}{c}\frac{2_1}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c2/m11$	L18
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cm2e$ $(\mathbf{a}/4)$	L36
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cm11$	L13
(100)	**b**	**c**	**a**	*Bbcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbam$	L44
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $(\mathbf{a}'/4)$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(010)	**c**	**a**	**b**	*Abma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmn$	L42
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbma$ $(\mathbf{b}'/4)$	L45
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24

*New symbol. Old symbol: *Cmca*.

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No. 65 *Cmmm* D_{2h}^{19}

$$\mathcal{G} = C\frac{2}{m}\frac{2}{m}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmmm*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*cmmm*	L47
					$[s\mathbf{d}, -s\mathbf{d}]$	*cmm*2	L26
(100)	**b**	**c**	**a**	*Bmmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmmm*	L37
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmma* $(\mathbf{a}'/4)$	L41
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pmm*2	L23
(010)	**c**	**a**	**b**	*Ammm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmmm*	L37
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmmb* $(\mathbf{b}'/4)$	L41
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pmm*2	L23

No. 66 *Cccm* D_{2h}^{20}

$$\mathcal{G} = C\frac{2}{c}\frac{2}{c}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cccm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p}112/m$	L06
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*c*222	L22
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03
(100)	**b**	**c**	**a**	*Bbmb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbmb*	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbmn* $(\mathbf{a}'/4)$	L42
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pbm*2 $(\mathbf{b}'/4)$	L24
(010)	**c**	**a**	**b**	*Amaa*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmaa*	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pman* $(\mathbf{b}'/4)$	L42
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pma*2 $(\mathbf{a}'/4)$	L24

No. 67* *Cmme* D_{2h}^{21}

$$\mathcal{G} = C\frac{2}{m}\frac{2}{m}\frac{2}{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Cmma*	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	*cmme*	L48
					$[s\mathbf{d}, -s\mathbf{d}]$	*cmm*2 $(\mathbf{b}/4)$	L26
(100)	**b**	**c**	**a**	*Bmcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmam*	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmaa* $(\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pma*2	L24
(010)	**c**	**a**	**b**	*Abmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbmb*	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbmm* $(\mathbf{b}'/4)$	L40
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	*pbm*2 $(\mathbf{b}'/4)$	L24

*New symbol. Old symbol: *Cmma*.

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No. 68* *Ccce* D_{2h}^{22}

$\mathcal{G} = C\frac{2}{c}\frac{2}{c}\frac{2}{a}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ccca* $[(\mathbf{b}+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*c*222	L22
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/n$ (**a**/4 or **b**/4)	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03
(100)	**b**	**c**	**a**	*Bbcb* $[(\mathbf{a}'+\mathbf{b}')/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pban* $[(\mathbf{a}'+\mathbf{b}')/4]$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbab* ($\mathbf{b}'$/4)	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2	L25
(010)	**c**	**a**	**b**	*Abaa* $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pban* $[(\mathbf{a}'+\mathbf{b}')/4]$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbaa* ($\mathbf{a}'$/4)	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2	L25

*New symbol. Old symbol: *Ccca*.

No. 68* *Ccce* D_{2h}^{22}

$\mathcal{G} = C\frac{2}{c}\frac{2}{c}\frac{2}{a}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ccca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{p}112/n$	L07
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*c*222 (**b**/4)	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$ (**a**/4 or **b**/4)	L03
(100)	**b**	**c**	**a**	*Bbcb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pban*	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbab* ($\mathbf{a}'$/4)	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2 $[(\mathbf{a}'+\mathbf{b}')/4]$	L25
(010)	**c**	**a**	**b**	*Abaa*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbaa*	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pban* ($\mathbf{b}'$/4)	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2 ($\mathbf{a}'$/4)	L25

*New symbol. Old symbol: *Ccca*.

No. 69 *Fmmm* D_{2h}^{23}

$\mathcal{G} = F\frac{2}{m}\frac{2}{m}\frac{2}{m}$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Fmmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*cmmm*	L47
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*cmme* ($\mathbf{b}'$/4)	L48
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*cmm*2	L26

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No. 70 *Fddd* D_{2h}^{24}

$\mathcal{G} = F\frac{2}{d}\frac{2}{d}\frac{2}{d}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Fddd* ($\boldsymbol{\tau}/8$)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}; \frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*c*222 *c*222 $[(\mathbf{a}'+\mathbf{b}')/4]$	 L22
(100)	**b**	**c**	**a**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}; \frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}112/b$ $[(\mathbf{a}'+\mathbf{b}')/8]$ $\widehat{p}112/a$ $[(3\mathbf{a}'+\mathbf{b}')/8$ or $(\mathbf{a}'+3\mathbf{b}')/8]$	 L07 L07
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d}; (\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$	L03

$\boldsymbol{\tau} = \mathbf{a}' + \mathbf{b}' + \mathbf{d}$.

No. 70 *Fddd* D_{2h}^{24}

$\mathcal{G} = F\frac{2}{d}\frac{2}{d}\frac{2}{d}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Fddd*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}; \frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/b$ $\widehat{p}112/a$ ($\mathbf{a}'/4$ or $\mathbf{b}'/4$)	L07 L07
(100)	**b**	**c**	**a**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}; \frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	*c*222 $[(\mathbf{a}'+\mathbf{b}')/8]$ *c*222 $[3(\mathbf{a}'+\mathbf{b}')/8]$	 L22 L22
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d}; (\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ $[(\mathbf{a}'+\mathbf{b}')/8]$	 L03

No. 71 *Immm* D_{2h}^{25}

$\mathcal{G} = I\frac{2}{m}\frac{2}{m}\frac{2}{m}$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Immm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmmm*	L37
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmmn* $[(\mathbf{a}'+\mathbf{b}')/4]$	L46
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pmm*2	L23

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No. 72 *Ibam* D_{2h}^{26}

$$\mathcal{G} = I\,{}^{2}_{b}\,{}^{2}_{a}\,{}^{2}_{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ibam*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbam*	L44
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pban* $[(\mathbf{a}+\mathbf{b})/4]$	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2	L25
(100)	**b**	**c**	**a**	*Icma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbmb*	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbma* $[(\mathbf{a}'+\mathbf{b}')/4]$	L45
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pbm*2 $(\mathbf{b}'/4)$	L24
(010)	**c**	**a**	**b**	*Imcb*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmaa*	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmab* $[(\mathbf{a}'+\mathbf{b}')/4]$	L45
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pma*2 $(\mathbf{a}'/4)$	L24

No. 73 *Ibca* D_{2h}^{27}

$$\mathcal{G} = I\,{}^{2_1}_{b}\,{}^{2_1}_{c}\,{}^{2}_{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Ibca*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbab*	L43
(100)	**b**	**c**	**a**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbaa* $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
(010)	**c**	**a**	**b**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2 $(\mathbf{b}'/4)$	L25

No. 74 *Imma* D_{2h}^{28}

$$\mathcal{G} = I\,{}^{2_1}_{m}\,{}^{2_1}_{m}\,{}^{2_1}_{a}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	*Imma*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmmb*	L41
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmma* $[(\mathbf{a}+\mathbf{b})/4]$	L41
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pmm*2 $(\mathbf{b}/4)$	L23
(100)	**b**	**c**	**a**	*Imcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmam*	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pman* $[(\mathbf{a}'+\mathbf{b}')/4]$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pma*2	L24
(010)	**c**	**a**	**b**	*Ibmm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pbmn*	L42
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pbmm* $[(\mathbf{a}'+\mathbf{b}')/4]$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pbm*2 $[(\mathbf{a}'+\mathbf{b}')/4]$	L24

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Auxiliary tables for Laue class D_{2h} – *mmm*

Centring types *P* and *I*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\overline{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(n0\overline{m})$	$\mathbf{b}$	$n\mathbf{c}+m\mathbf{a}$	$-p\mathbf{c}+q\mathbf{a}$			

Arithmetic class 222*P*

Serial No.	16	17	18	19
Group type	D_2^1	D_2^2	D_2^3	D_2^4
Group	$P222$	$P222_1$	$P2_12_12$	$P2_12_12_1$
$(mn0)$ $(\overline{m}n0)$	$P112$	$P112_1$	$P112$	$P112_1$ $(\mathbf{a}/4)$
$(0mn)$ $(0\overline{m}n)$		$P112$	$P112_1$ $(\mathbf{b}/4)$	$P112_1$ $(\mathbf{b}/4)$
$(n0m)$ $(n0\overline{m})$		$P112$ $(\mathbf{c}/4)$	$P112_1$ $(\mathbf{a}/4)$	$P112_1$ $(\mathbf{c}/4)$

Arithmetic class *mm*2*P*

Serial No.	25	26	27	28	29	30	31	32	33	34
Group type	C_{2v}^1	C_{2v}^2	C_{2v}^3	C_{2v}^4	C_{2v}^5	C_{2v}^6	C_{2v}^7	C_{2v}^8	C_{2v}^9	C_{2v}^{10}
Group	$Pmm2$	$Pmc2_1$	$Pcc2$	$Pma2$	$Pca2_1$	$Pnc2$	$Pmn2_1$	$Pba2$	$Pna2_1$	$Pnn2$
$(mn0)$ $(\overline{m}n0)$	$P112$	$P112_1$	$P112$	$P112$	$P112_1$	$P112$	$P112_1$ $(\mathbf{a}/4)$	$P112$	$P112_1$	$P112$
$(0mn)$ $(0\overline{m}n)$	$P11m$	$P11m$	$P11b$	$P11m$ $(\mathbf{a}/4)$	$P11b$ $(\mathbf{a}/4)$	$P11n$	$P11m$	$P11a$ $(\mathbf{a}/4)$	$P11n$ $(\mathbf{a}/4)$	$P11n$ $(\mathbf{a}/4)$
$(n0m)$ $(n0\overline{m})$		$P11a$	$P11a$	$P11b$	$P11b$	$P11a$ $(\mathbf{b}/4)$	$P11n$	$P11b$ $(\mathbf{b}/4)$	$P11b$ $(\mathbf{b}/4)$	$P11n$ $(\mathbf{b}/4)$

Arithmetic classes 222*I*, *mm*2*I* and *mmmI*

Serial No.	23	24	44	45	46	71	72	73	74
Group type	D_2^8	D_{2v}^9	C_{2v}^{20}	C_{2v}^{21}	C_{2v}^{22}	D_{2h}^{25}	D_{2h}^{26}	D_{2h}^{27}	D_{2h}^{28}
Group	$I222$	$I2_12_12_1$	$Imm2$	$Iba2$	$Ima2$	$Immm$	$Ibam$	$Ibca$	$Imma$
$(mn0)$ $(\overline{m}n0)$	$I112$	$I112$ $(\mathbf{b}/4)$	$I112$	$I112$	$I112$	$I112/m$	$I112/m$	$I112/b$	$I112/b$
$(0mn)$ $(0\overline{m}n)$		$I112$ $(\mathbf{c}/4)$	$I11m$	$I11b$	$I11m$ $(\mathbf{a}/4)$		$I112/b$		$I112/m$
$(n0m)$ $(n0\overline{m})$		$I112$ $(\mathbf{a}/4)$		$I11a$	$I11b$		$I112/a$		$I112/m$ $[(\mathbf{a}+\mathbf{b}+\mathbf{c})/4]$

Arithmetic class *mmmP*

Serial No. Group type Group	47 D_{2h}^{1} *Pmmm*	48 D_{2h}^{2} *Pnnn*		49 D_{2h}^{3} *Pccm*	50 D_{2h}^{4} *Pban*	
		Origin 1	Origin 2		Origin 1	Origin 2
$(mn0)$ $(\overline{m}n0)$	$P112/m$	$P112/n$ $[(\mathbf{a}+\mathbf{b}+\mathbf{c})/4]$	$P112/n$	$P112/m$	$P112/n$ $[(\mathbf{a}+\mathbf{b})/4]$	$P112/n$
$(0mn)$ $(0\overline{m}n)$				$P112/b$	$P112/a$ $[(\mathbf{a}+\mathbf{b})/4]$	$P112/a$
$(n0m)$ $(n0\overline{m})$				$P112/a$	$P112/b$ $[(\mathbf{a}+\mathbf{b})/4]$	$P112/b$

Serial No. Group type Group	51 D_{2h}^{5} *Pmma*	52 D_{2h}^{6} *Pnna*	53 D_{2h}^{7} *Pmna*	54 D_{2h}^{8} *Pcca*	55 D_{2h}^{9} *Pbam*	56 D_{2h}^{10} *Pccn*
$(mn0)$ $(\overline{m}n0)$	$P112/a$	$P112/a$	$P112_1/a$	$P112/a$	$P112/m$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$P112_1/m$	$P112/n$	$P112/m$	$P112_1/b$	$P112_1/a$	$P112_1/b$
$(n0m)$ $(n0\overline{m})$	$P112/m$	$P112_1/n$	$P112/n$	$P112/a$	$P112_1/b$	$P112_1/a$

Serial No. Group type Group	57 D_{2h}^{11} *Pbcm*	58 D_{2h}^{12} *Pnnm*	59 D_{2h}^{13} *Pmmn*		60 D_{2h}^{14} *Pbcn*	61 D_{2h}^{15} *Pbca*	62 D_{2h}^{16} *Pnma*
			Origin 1	Origin 2			
$(mn0)$ $(\overline{m}n0)$	$P112_1/m$	$P112/m$	$P112/n$ $[(\mathbf{a}+\mathbf{b})/4]$	$P112/n$	$P112_1/n$	$P112_1/a$	$P112_1/a$
$(0mn)$ $(0\overline{m}n)$	$P112/a$	$P112_1/n$	$P112_1/m$ $[(\mathbf{a}+\mathbf{b})/4]$	$P112_1/m$	$P112_1/a$		$P112_1/n$
$(n0m)$ $(n0\overline{m})$	$P112_1/a$				$P112/a$		$P112_1/m$

Centring type *C*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(hk0)$ $(\overline{h}k0)$	$\mathbf{c}$ $\mathbf{c}$	$n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}$ $n\widehat{\mathbf{a}}+m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$ $-p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$
h even, k odd or h odd, k even $\Rightarrow n=h+k, m=h-k$ h, k odd $\Rightarrow n=(h+k)/2, m=(h-k)/2$						
$(0mn)$ $(0\overline{m}n)$	$\mathbf{a}$ $\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$ $n\mathbf{b}+m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$ $-p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(n0m)$ $(n0\overline{m})$	$\mathbf{b}$ $\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$ $n\mathbf{c}+m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$ $-p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$

Arithmetic classes 222*C* and *mm*2*C*

Serial No.	20	21	35	36	37
Group type	D_2^5	D_2^6	C_{2v}^{11}	C_{2v}^{12}	C_{2v}^{13}
Group	$C222_1$	$C222$	$Cmm2$	$Cmc2_1$	$Ccc2$
$(hk0)$ $(\overline{h}k0)$	$P112_1$	$P112$	$P112$	$P112_1$	$P112$
$(0mn)$ $(0\overline{m}n)$	$B112$	$B112$	$B11m$	$B11m$	$B11b$
$(n0m)$ $(n0\overline{m})$	$A112$ $(\mathbf{c}/4)$	$A112$	$A11m$	$A11a$	$A11a$

Arithmetic class *mmm*C

Serial No.	63	64	65	66	67	68	
Group type	D_{2h}^{17}	D_{2h}^{18}	D_{2h}^{19}	D_{2h}^{20}	D_{2h}^{21}	D_{2h}^{22}	
Group	$Cmcm$	$Cmce$	$Cmmm$	$Cccm$	$Cmme$	$Ccce$	
						Origin 1	Origin 2
$(hk0)$ $(\overline{h}k0)$	$P112_1/m$	$P112_1/n$	$P112/m$	$P112/m$	$P112/n$	$P112/n$ $[(\mathbf{b}+\mathbf{c})/4]$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$B112/m$	$B112/m$	$B112/m$	$B112/b$	$B112/m$	$B112/n$ $[(\mathbf{a}+\mathbf{c})/4]$	$B112/n$
$(n0m)$ $(n0\overline{m})$	$A112/a$	$A112/n$	$A112/m$	$A112/a$	$A112/m$ $[(\mathbf{a}+\mathbf{b})/4]$	$A112/a$ $[(\mathbf{b}+\mathbf{c})/4]$	$A112/a$

Centring type *A*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(0kl)$	$\mathbf{a}$	$n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$
$(\overline{k}l0)$	$\mathbf{a}$	$n\widehat{\mathbf{a}}+m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$			
k even, l odd or k odd, l even $\Rightarrow n=k+l, m=k-l$ k, l odd $\Rightarrow n=(k+l)/2, m=(k-l)/2$						
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(n0\overline{m})$	$\mathbf{b}$	$n\mathbf{c}+m\mathbf{a}$	$-p\mathbf{c}+q\mathbf{a}$			

Arithmetic class *mm*2*A*

Serial No.	38	39	40	41
Group type	C_{2v}^{14}	C_{2v}^{15}	C_{2v}^{16}	C_{2v}^{17}
Group	$Amm2$	$Aem2$	$Ama2$	$Aea2$
$(mn0)$ $(\overline{m}n0)$	$A112$	$A112$	$A112$	$A112$
$(0kl)$ $(0\overline{k}l)$	$P11m$	$P11n$	$P11m$ $(\mathbf{a}/4)$	$P11n$ $(\mathbf{a}/4)$
$(n0m)$ $(n0\overline{m})$	$B11m$	$B11m$ $(\mathbf{b}/4)$	$B11b$	$B11b$ $(\mathbf{b}/4)$

Centring type *F*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(hk0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$
$(\bar{h}k0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}}+m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$			
$(0hk)$	$\mathbf{a}$	$n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$
$(0\bar{h}k)$	$\mathbf{a}$	$n\widehat{\mathbf{a}}+m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$			
$(k0h)$	$\mathbf{b}$	$n\widehat{\mathbf{a}}-m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$
$(k0\bar{h})$	$\mathbf{b}$	$n\widehat{\mathbf{a}}+m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}}+q\widehat{\mathbf{b}}$			

h even, k odd or h odd, k even $\Rightarrow n=h+k$, $m=h-k$
h, k odd $\Rightarrow n=(h+k)/2$, $m=(h-k)/2$

Arithmetic classes $222F$, $mm2F$ and $mmmF$

Serial No.	22	42	43	69	70	
Group type	D_2^7	C_{2v}^{18}	C_{2v}^{19}	D_{2h}^{23}	D_{2h}^{24}	
Group	$F222$	$Fmm2$	$Fdd2$	$Fmmm$	$Fddd$	
					Origin 1	Origin 2
$(hk0)$ $(\bar{h}k0)$	$I112$	$I112$	$I112$	$I112/m$	$I112/b$ $[(\mathbf{a}+\mathbf{b}+\mathbf{c})/8]$	$I112/b$
$(0hk)$ $(0\bar{h}k)$		$I11m$	$I11b$ $(\mathbf{a}/8)$			
$(k0h)$ $(k0\bar{h})$						

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 75, p. 470.

Laue class C_{4h} – $4/m$

Geometric class C_4 – 4

No. 75 $P4$ C_4^1

$$\mathcal{G} = P4$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$P4$	$s\mathbf{d}$	$p4$ L49

No. 76 $P4_1$ C_4^2

$$\mathcal{G} = P4_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$P4_1$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$p1$ L01

No. 77 $P4_2$ C_4^3

$$\mathcal{G} = P4_2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$P4_2$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$ L03

No. 78 $P4_3$ C_4^4

$$\mathcal{G} = P4_3$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$P4_3$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$p1$ L01

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No. 79 $I4$ C_4^5

$$\mathcal{G} = I4$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$I4$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p4$ L49

No. 80 $I4_1$ C_4^6

$$\mathcal{G} = I4_1$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$I4_1$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$p112$ L03

Geometric class $S_4 - \overline{4}$

No. 81 $P\overline{4}$ S_4^1

$$\mathcal{G} = P\overline{4}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$P\overline{4}$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p\overline{4}$ L50
			$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ L03

No. 82 $I\overline{4}$ S_4^2

$$\mathcal{G} = I\overline{4}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(001)	**a** **b** **c**	$I\overline{4}$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{4}$ L50
			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\overline{4}$ ($\mathbf{a}/2$ or $\mathbf{b}/2$) L50
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ L03

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Geometric class $C_{4h}-4/m$

No. 83 $P4/m$ C_{4h}^1

$$\mathcal{G} = P4/m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4/m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$ $[s\mathbf{d}, -s\mathbf{d}]$	$p4/m$ $p4$	L51 L49

No. 84 $P4_2/m$ C_{4h}^2

$$\mathcal{G} = P4_2/m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4_2/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112/m$ $p112$	L06 L03

No. 85 $P4/n$ C_{4h}^3

$$\mathcal{G} = P4/n \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4/n$ (origin 1)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$ $[s\mathbf{d}, -s\mathbf{d}]$	$p4/n$ ($\mathbf{a}/2$ or $\mathbf{b}/2$) $p112$	L52 L03

No. 85 $P4/n$ C_{4h}^3

$$\mathcal{G} = P4/n \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4/n$ (origin 2)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$ $[s\mathbf{d}, -s\mathbf{d}]$	$p4/n$ $[(\mathbf{a}+\mathbf{b})/4]$ $p112$ $[(\mathbf{a}+\mathbf{b})/4]$	L52 L03

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No. 86 $P4_2/n$ C_{4h}^4

$\mathcal{G} = P4_2/n$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4_2/n$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}$	L50
			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $[(\mathbf{a}+\mathbf{b})/4]$	L07
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 86 $P4_2/n$ C_{4h}^4

$\mathcal{G} = P4_2/n$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$P4_2/n$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}$ $[(\mathbf{a}+\mathbf{b})/4]$	L50
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}+\mathbf{b})/4]$	L03

No. 87 $I4/m$ C_{4h}^5

$\mathcal{G} = I4/m$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$I4/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/m$	L51
			$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/n$	L52
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 88 $I4_1/a$ C_{4h}^6

$\mathcal{G} = I4_1/a$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$I4_1/a$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{4}$	L50
			$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L50
			$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p112/b$ ($\mathbf{b}/4$)	L07
			$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p112/a$ ($\mathbf{a}/4$)	L07
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
			$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p112$	L03

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No. 88 $I4_1/a$ C_{4h}^6

$\mathcal{G} = I4_1/a$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a** **b** **c**	$I4_1/a$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p112/b$	L07
			$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a\ [(\mathbf{a}+\mathbf{b})/4]$	L07
			$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}\ (\mathbf{b}/4)$	L50
			$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}\ (3\mathbf{b}/4)$	L50
			$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
			$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p112\ (\mathbf{b}/4)$	L03

Auxiliary tables for Laue class $C_{4h}-4/m$

Centring types *P* and *I*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	**c**	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	**a**	**b**	**c**
$(\bar{n}m0)$	**c**	$m\mathbf{a}+n\mathbf{b}$	$-q\mathbf{a}+p\mathbf{b}$			

Arithmetic classes $4P$ and $4I$

Serial No.	75	76	77	78	79	80
Group type	C_4^1	C_4^2	C_4^3	C_4^4	C_4^5	C_4^6
Group	$P4$	$P4_1$	$P4_2$	$P4_3$	$I4$	$I4_1$
$(mn0)$ $(\bar{m}n0)$	$P112$	$P112_1$	$P112$	$P112_1$	$I112$	$I112$

Arithmetic classes $\bar{4}P$ and $\bar{4}$

Serial No.	81	82
Group type	S_4^1	S_4^2
Group	$P\bar{4}$	$I\bar{4}$
$(mn0)$ $(\bar{m}n0)$	$P112$	$I112$

Arithmetic class $4/mP$

Serial No.	83	84	85		86	
Group type	C_{4h}^1	C_{4h}^2	C_{4h}^3		C_{4h}^4	
Group	$P4/m$	$P4_2/m$	$P4/n$		$P4_2/n$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\bar{m}n0)$	$P112/m$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b})/4$	$P112/n$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$

Arithmetic class $4/mI$

Serial No.	87	88	
Group type	C_{4h}^5	C_{4h}^6	
Group	$I4/m$	$I4_1/a$	
		Origin 1	Origin 2
$(mn0)$	$I112/m$	$I112/b$	$I112/b$
$(\overline{m}n0)$		$(\mathbf{b}/4+\mathbf{c}/8)$	

Laue class $D_{4h}-4/mmm$

Geometric class D_4 – 422

No. 89 $P422$ D_4^1

$$\mathcal{G}=P422$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P422$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p422$	L53
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4$	L49
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$P222$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p222$	L19
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\overline{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 90 $P42_12$ D_4^2

$$\mathcal{G}=P42_12$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P42_12$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p42_12$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L54
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L49
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$P2_122_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\overline{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 91 $P4_122$ D_4^3

$$\mathcal{G} = P4_122$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p121$	L08
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{c}211$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{c}121$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(100)	**b**	**c**	**a**	$P22_12$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p22_12$ $(\mathbf{b}'/4)$	L20
				$(\mathbf{b}'/4)$	$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03
(010)	$-\mathbf{a}$	**c**	**b**	$P22_12$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p22_12$	L20
					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(3\mathbf{b}'/8)$	L20
				$(\mathbf{b}'/8)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/8)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/8)$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/8)$	L20
				$(\mathbf{b}'/8)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/8)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/8)$	L03

No. 92 $P4_12_12$ D_4^4

$$\mathcal{G} = P4_12_12$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_12_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{c}121$	L10
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}211$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p12_11$ $(\mathbf{a}/4)$	L09
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_111$ $(\mathbf{b}/4)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(100)	**b**	**c**	**a**	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_11$	L09
				$(3\mathbf{b}'/8 + \mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/8)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	$-\mathbf{a}$	**c**	**b**	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_11$	L09
				$(\mathbf{b}'/8 + \mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/8)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/4)$	L20
				$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/4)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

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No. 93 $P4_222$ D_4^5

$$\mathcal{G} = P4_222$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$P222$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p222$	L19
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{b}'/4)$	L19
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ $(\mathbf{b}'/4)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

No. 94 $P4_22_12$ D_4^6

$$\mathcal{G} = P4_22_12$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}222$	L22
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$P2_122_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$	$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 95 $P4_322$ D_4^7

$$\mathcal{G} = P4_322$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_322$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p121$	L08
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{c}121$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{c}211$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(100)	**b**	**c**	**a**	$P22_12$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p22_12$ $(\mathbf{b}'/4)$	L20
				$(\mathbf{b}'/4)$	$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03
(010)	$-\mathbf{a}$	**c**	**b**	$P22_12$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p22_12$	L20
					$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/8)$	L20
				$(\mathbf{b}'/8)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/8)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/8)$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/8)$	L20
				$(\mathbf{b}'/8)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/8)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/8)$	L03

No. 96 $P4_32_12$ D_4^8

$$\mathcal{G} = P4_32_12$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_32_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{c}121$	L10
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}211$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p2_111$ $(\mathbf{b}/4)$	L09
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p12_11$ $(\mathbf{a}/4)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(100)	**b**	**c**	**a**	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_11$	L09
				$(\mathbf{b}'/8 + \mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/8)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(010)	$-\mathbf{a}$	**c**	**b**	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12_11$	L09
				$(3\mathbf{b}'/8 + \mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/8)$	L09
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$B22_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/4)$	L20
				$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{b}'/4)$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

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No. 97 $I422$ D_4^9

$$\mathcal{G} = I422$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I422$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p422$	L53
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p42_12$	L54
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	**b**	**c**	**a**	$I222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222\ [(\mathbf{a}'+\mathbf{b}')/4]$	L22
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03

No. 98 $I4_122$ D_4^{10}

$$\mathcal{G} = I4_122$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}$;	$\widehat{c}222$	L22
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L22
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}$;	$p22_12$	L20
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d}$,		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L20
				($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L03
(010)	$-\mathbf{a}$	**c**	**b**	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/4+3\mathbf{b}'/8$)	L20
				($\mathbf{a}'/4 + \mathbf{b}'/8$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ ($\mathbf{a}'/4+3\mathbf{b}'/8$)	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222\ [(\mathbf{a}'+\mathbf{b}')/4]$	L22
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03

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Geometric class $C_{4v} - 4mm$

No. 99 $P4mm$ C_{4v}^1

$$\mathcal{G} = P4mm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4mm$	$s\mathbf{d}$	$p4mm$	L55
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pm2m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pm2m$	L27
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2a$ $(\mathbf{a}'/4)$	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 100 $P4bm$ C_{4v}^2

$$\mathcal{G} = P4bm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4bm$	$s\mathbf{d}$	$p4bm$	L55
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pc2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2a$	L31
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2m$ $(\mathbf{a}'/4)$	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11

No. 101 $P4_2cm$ C_{4v}^3

$$\mathcal{G} = P4_2cm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2cm$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pb2b$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pb2b$	L30
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2a$ $(\mathbf{a}'/4)$	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

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No. 102 $P4_2nm$ C_{4v}^4

$$\mathcal{G} = P4_2nm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2nm$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	**b**	**c**	**a**	$Pn2n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2a$ $(\mathbf{a}'/4)$	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 103 $P4cc$ C_{4v}^5

$$\mathcal{G} = P4cc$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4cc$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	**b**	**c**	**a**	$Pb2b$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pb2b$	L30
(010)	$-\mathbf{a}$	**c**	**b**		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2n$ $(\mathbf{a}'/4)$	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12

No. 104 $P4nc$ C_{4v}^6

$$\mathcal{G} = P4nc$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4nc$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	**b**	**c**	**a**	$Pn2n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2n$	L34
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

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No. 105 $P4_2mc$ C_{4v}^7

$$\mathcal{G} = P4_2mc$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2mc$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pm2m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pm2m$	L27
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2n$ $(\mathbf{a}'/4)$	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12

No. 106 $P4_2bc$ C_{4v}^8

$$\mathcal{G} = P4_2bc$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2bc$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pc2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2n$	L34
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

No. 107 $I4mm$ C_{4v}^9

$$\mathcal{G} = I4mm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I4mm$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p4mm$	L55
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Im2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Fm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cm2m$	L35
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cm2e$ $(\mathbf{a}'/4)$	L36
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cm11$	L13

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No. 108 $I4cm$ C_{4v}^{10}

$$\mathcal{G} = I4cm$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4cm$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p4bm$	L56
(100)	**b**	**c**	**a**	$Ic2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$ $(\mathbf{a}'/4)$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cm2e$	L36
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cm2m$ $(\mathbf{a}'/4)$	L35
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cm11$ $(\mathbf{a}'/4)$	L13

No. 109 $I4_1md$ C_{4v}^{11}

$$\mathcal{G} = I4_1md$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_1md$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d},$ $(s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Im2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ $(\mathbf{a}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11b$	L07
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11a$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
				$[(\mathbf{a}'+\mathbf{d})/4]$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ $(\mathbf{a}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11a$ $(\mathbf{a}'/4)$	L07
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11b$ $(\mathbf{a}'/4)$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01

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No. 110 $I4_1cd$ C_{4v}^{12}

$$\mathcal{G} = I4_1cd$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I4_1cd$	$[s\mathbf{d}, (s+\frac{1}{4})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{3}{4})\mathbf{d}]$	$pba2$	L25
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Ic2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$ $(\mathbf{a}'/4)$	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
				$[(\mathbf{a}'+\mathbf{d})/4]$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ $(\mathbf{a}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11a$ $(\mathbf{a}'/4)$	L05
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11b$ $(\mathbf{a}'/4)$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ $(\mathbf{a}'/4)$	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11b$	L05
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11a$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p1$	L01

Geometric classes $D_{2d} - \bar{4}2m$ and $\bar{4}m2$

No. 111 $P\bar{4}2m$ D_{2d}^{1}

$$\mathcal{G} = P\bar{4}2m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}2m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p\bar{4}2m$	L57
					$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$P222$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p222$	L19
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2a$ $(\mathbf{a}'/4)$	L31
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

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No. 112 $P\bar{4}2c$ D_{2d}^2

$$\mathcal{G} = P\bar{4}2c$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P\bar{4}2c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}$	L50
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$P222$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p222$ $(\mathbf{b}'/4)$	L19
(010)	$-\mathbf{a}$	**c**	**b**	$(\mathbf{b}'/4)$	$[s\mathbf{d}, -s\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2n$ $(\mathbf{a}'/4)$	L34
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12

No. 113 $P\bar{4}2_1m$ D_{2d}^3

$$\mathcal{G} = P\bar{4}2_1m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P\bar{4}2_1m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p\bar{4}2_1m$	L58
					$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{c}mm2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L26
(100)	**b**	**c**	**a**	$P2_122_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2a$	L31
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2m$ $(\mathbf{a}'/4)$	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11

No. 114 $P\bar{4}2_1c$ D_{2d}^4

$$\mathcal{G} = P\bar{4}2_1c$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P\bar{4}2_1c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}$	L50
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$P2_122_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	**c**	**b**	$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_111$ $(\mathbf{b}'/4)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bb2b$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2n$	L34
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12

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No. 115 $P\bar{4}m2$ D_{2d}^5

$$\mathcal{G} = P\bar{4}m2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}m2$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{4}m2$	L59
					$[s\mathbf{d}, -s\mathbf{d}]$	$pmm2$	L23
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pm2m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pm2m$	L27
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 116 $P\bar{4}c2$ D_{2d}^6

$$\mathcal{G} = P\bar{4}c2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}c2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}$	L50
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pb2b$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pb2b$	L30
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{b}'/4)$	L19
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$(\mathbf{b}'/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ $(\mathbf{b}'/4)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03

No. 117 $P\bar{4}b2$ D_{2d}^7

$$\mathcal{G} = P\bar{4}b2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}b2$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{4}b2$	L60
					$[s\mathbf{d}, -s\mathbf{d}]$	$pba2$	L25
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pc2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11a$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/4)$	L20
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $(\mathbf{a}'/4)$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03

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No. 118 $P\bar{4}n2$ D_{2d}^{8}

$$\mathcal{G} = P\bar{4}n2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P\bar{4}n2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}$	L50
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$Pn2n$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$B222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L20
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L03

No. 119 $I\bar{4}m2$ D_{2d}^{9}

$$\mathcal{G} = I\bar{4}m2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I\bar{4}m2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}m2$	L59
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L59
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Im2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03

No. 120 $I\bar{4}c2$ D_{2d}^{10}

$$\mathcal{G} = I\bar{4}c2$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I\bar{4}c2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}b2$	L60
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(100)	**b**	**c**	**a**	$Ic2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2_1a$ ($\mathbf{a}'/4$)	L33
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$ ($\mathbf{b}'/4$)	L22
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	($\mathbf{b}'/4$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ ($\mathbf{a}'/4$)	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$ ($\mathbf{b}'/4$)	L03

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No. 121 $I\bar{4}2m$ D_{2d}^{11}

$$\mathcal{G} = I\bar{4}2m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I\bar{4}2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}2m$	L57
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2_1m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L58
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	**b**	**c**	**a**	$I222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fm2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cm2m$	L35
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cm2a$ ($\mathbf{a}'/4$)	L36
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$cm11$	L13

No. 122 $I\bar{4}2d$ D_{2d}^{12}

$$\mathcal{G} = I\bar{4}2d$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I\bar{4}2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{4}$	L50
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L50
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p22_12$	L20
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p112$	L03
(100)	**b**	**c**	**a**	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L20
				($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L03
(010)	$-\mathbf{a}$	**c**	**b**	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/4+3\mathbf{b}'/8$)	L20
				($\mathbf{a}'/4 + \mathbf{b}'/8$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ ($\mathbf{a}'/4+3\mathbf{b}'/8$)	L20
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ ($\mathbf{a}'/4$)	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11b$	L05
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11a$	L05
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Fd2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d},$	$c121$	L10
				$[(\mathbf{a}' + \mathbf{d})/4]$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c121$ ($\mathbf{a}'/4$)	L10
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d},$	$\widehat{p}11a$ ($\mathbf{a}'/4$)	L05
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}11b$ ($\mathbf{a}'/4$)	L05
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01

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Geometric class $D_{4h}-4/mmm$

No. 123 $P4/mmm$ D_{4h}^1

$$\mathcal{G} = P\frac{4}{m}\frac{2}{m}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/mmm$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p4/mmm$	L61
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4mm$	L55
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pmmm$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pmmm$	L37
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pmm2$	L23
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmma$ $(\mathbf{a}'/4)$	L41
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23

No. 124 $P4/mcc$ D_{4h}^2

$$\mathcal{G} = P\frac{4}{m}\frac{2}{c}\frac{2}{c}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/mcc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/m$	L51
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p422$	L53
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pbmb$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$pbmb$	L38
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bbmb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmb$	L38
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmn$ $(\mathbf{a}'/4)$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24

No. 125 $P4/nbm$ D_{4h}^3

$$\mathcal{G} = P\frac{4}{n}\frac{2}{b}\frac{2}{m} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/nbm$ (origin 1)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p4/nbm$	L62
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4bm$	L56
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pcna$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $(\mathbf{a}'/4)$	L07
					$[\pm s\mathbf{d}\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bmcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$ $(\mathbf{a}'/4)$	L38
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$(\mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24

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No. 125 $P4/nbm$ D_{4h}^3

$$\mathcal{G} = P\frac{4}{n}\frac{2}{b}\frac{2}{m} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/nbm$ (origin 2)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p4/nbm\ [(\mathbf{a}+\mathbf{b})/4]$	L62
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4bm\ [(\mathbf{a}+\mathbf{b})/4]$	L56
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pcna$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222\ (\mathbf{a}'/4)$	L19
					$[\pm s\mathbf{d}\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/4)$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bmcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa\ (\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$Bmcm$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam\ (\mathbf{a}'/4)$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2\ (\mathbf{a}'/4)$	L24

No. 126 $P4/nnc$ D_{4h}^4

$$\mathcal{G} = P\frac{4}{n}\frac{2}{n}\frac{2}{c} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/nnc$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p422$	L53
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/n$	L52
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pnnn$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n\ [(\mathbf{a}'+\mathbf{b}')/4]$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban\ [(\mathbf{a}'+\mathbf{b}')/4]$	L39
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	or $Bbcb$ (or. 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab\ (\mathbf{b}'/4)$	L43
				$[(\mathbf{a}'+\mathbf{b}')/4]$	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25

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No. 126 $P4/nnc$ D_{4h}^4

$$\mathcal{G} = P\frac{4}{n}\frac{2}{n}\frac{2}{c} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/nnc$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/n$ $[(\mathbf{a}+\mathbf{b})/4]$	L52
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p422$ $[(\mathbf{a}+\mathbf{b})/4]$	L53
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$ $[(\mathbf{a}+\mathbf{b})/4]$	L49
(100)	**b**	**c**	**a**	$Pnnn$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{b}'+\mathbf{d})/4]$ or $Bbcb$ (or. 2) $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $(\mathbf{a}'/4)$	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{a}'+\mathbf{b}')/4]$ or $Bbcb$ (or. 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $(\mathbf{a}'/4)$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L25

No. 127 $P4/mbm$ D_{4h}^5

$$\mathcal{G} = P\frac{4}{m}\frac{2_1}{b}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/mbm$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p4/mbm$	L63
					$[s\mathbf{d}, -s\mathbf{d}]$	$p4bm$	L56
(100)	**b**	**c**	**a**	$Pcma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ma$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmmm$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmma$	L41
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmm$ $(\mathbf{a}'/4)$	L37
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$ $(\mathbf{a}'/4)$	L23

No. 128 $P4/mnc$ D_{4h}^6

$$\mathcal{G} = P\frac{4}{m}\frac{2_1}{n}\frac{2}{c}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/mnc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/m$	L51
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p42_12$	L54
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(100)	**b**	**c**	**a**	$Pnmn$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbmb$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmn$	L42
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmb$ $(\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24

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No. 129 $P4/nmm$ D_{4h}^7

$\mathcal{G} = P\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/nmm$ (origin 1)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$ $[s\mathbf{d}, -s\mathbf{d}]$	$p4/nmm$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L64
						$p4mm$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L55
(100)	**b**	**c**	**a**	$Pmnm$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ ($\mathbf{a}'/4$)	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmcm$ ($\mathbf{d}/4$)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$ ($\mathbf{a}'/4$)	L38
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24

No. 129 $P4/nmm$ D_{4h}^7

$\mathcal{G} = P\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/nmm$ (origin 2)	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$ $[s\mathbf{d}, -s\mathbf{d}]$	$p4/nmm$ $[(\mathbf{a}+\mathbf{b})/4]$	L64
						$p4mm$ $[(\mathbf{a}+\mathbf{b})/4]$	L55
(100)	**b**	**c**	**a**	$Pmnm$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/m11$	L15
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2m$ ($\mathbf{a}'/4$)	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ ($\mathbf{a}'/4$)	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmcm$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$ ($\mathbf{a}'/4$)	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ ($\mathbf{a}'/4$)	L24
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bmcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa$ ($\mathbf{a}'/4$)	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24

No. 130 $P4/ncc$ D_{4h}^8

$\mathcal{G} = P\frac{4}{n}\frac{2_1}{c}\frac{2}{c}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/ncc$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/n$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L52
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p42_12$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L54
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L49
(100)	**b**	**c**	**a**	$Pbnb$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$	L30
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ ($\mathbf{a}'/4$)	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1) ($\mathbf{b}'/4$) or $Bbcb$ (or. 2) ($\mathbf{a}'/4$)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$ ($\mathbf{a}'/4$)	L39
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ ($\mathbf{b}'/4$)	L25

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No. 130 $P4/ncc$ D_{4h}^{8}

$$\mathcal{G} = P\frac{4}{n}\frac{2_1}{c}\frac{2}{c} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4/ncc$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/n$ $[(\mathbf{a}+\mathbf{b})/4]$	L52
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p42_12$ $[(\mathbf{a}+\mathbf{b})/4]$	L54
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$ $[(\mathbf{a}+\mathbf{b})/4]$	L49
(100)	**b**	**c**	**a**	$Pbnb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{a}'+\mathbf{b}')/4]$ or $Bbcb$ (or. 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $(\mathbf{a}'/4)$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L25
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{b}'+\mathbf{d})/4]$ or $Bbcb$ (or. 2) $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $(\mathbf{a}'/4)$	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25

No. 131 $P4_2/mmc$ D_{4h}^{9}

$$\mathcal{G} = P\frac{4_2}{m}\frac{2}{m}\frac{2}{c}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/mmc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$	L59
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Pmmm$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pmmm$	L37
(010)	$-\mathbf{a}$	**c**	**b**		$[s\mathbf{d}, -s\mathbf{d}]$	$pmm2$	L23
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbmb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmb$	L38
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmn$ $(\mathbf{a}'/4)$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24

No. 132 $P4_2/mcm$ D_{4h}^{10}

$$\mathcal{G} = P\frac{4_2}{m}\frac{2}{c}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/mcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}mmm$	L47
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2m$	L57
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	**b**	**c**	**a**	$Pbmb$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pbmb$	L38
(010)	$-\mathbf{a}$	**c**	**b**		$[s\mathbf{d}, -s\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmma$ $(\mathbf{a}'/4)$	L41
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23

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No. 133 $P4_2/nbc$ D_{4h}^{11}

$\mathcal{G} = P\frac{4_2}{n}\frac{2}{b}\frac{2}{c}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/nbc$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}b2$	L60
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $[(\mathbf{a}+\mathbf{b})/4]$	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(100)	**b**	**c**	**a**	$Pcna$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{b}'/4)$	L19
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/a$ $[(\mathbf{a}'+\mathbf{b}')/4)]$	L07
				$(\mathbf{b}'/4)$	$[\pm s\mathbf{d}\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{b}'/4)$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $(\mathbf{b}'/4)$	L39
				or $Bbcb$ (or. 2)	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{a}'/4)$	L25
				$[(\mathbf{b}'+\mathbf{d})/4]$			

No. 133 $P4_2/nbc$ D_{4h}^{11}

$\mathcal{G} = P\frac{4_2}{n}\frac{2}{b}\frac{2}{c}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/nbc$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$ $[(\mathbf{a}+3\mathbf{b})/4$	
						or $(3\mathbf{a}+\mathbf{b})/4]$	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $[(\mathbf{a}+\mathbf{b})/4]$	L25
(100)	**b**	**c**	**a**	$Pcna$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $(\mathbf{a}'/4)$	L19
					$[\pm s\mathbf{d}\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
				$[(\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $(\mathbf{a}'/4)$	L39
				or $Bbcb$ (or. 2)	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
				$[(\mathbf{a}'+\mathbf{d})/4]$			
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bbcb$ (or. 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
				$[(\mathbf{a}'+\mathbf{b}')/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $(\mathbf{a}'/4)$	L43
				or $Bbcb$ (or. 2)	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L25

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No. 134 $P4_2/nnm$ D_{4h}^{12}

$\mathcal{G} = P\frac{4_2}{n}\frac{2}{n}\frac{2}{m}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/nnm$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}2m$	L57
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}mme$ $[(\mathbf{a}+\mathbf{b})/4]$	L36
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	**b**	**c**	**a**	$Pnnn$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmcm$ $[(\mathbf{a}'+\mathbf{b}')/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L40
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa$ $(\mathbf{b}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24

No. 134 $P4_2/nnm$ D_{4h}^{12}

$\mathcal{G} = P\frac{4_2}{n}\frac{2}{n}\frac{2}{m}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/nnm$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}mme$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L36
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2m$ $[(\mathbf{a}+3\mathbf{b})/4$ or $(3\mathbf{a}+\mathbf{b})/4]$	L57
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$ $[(\mathbf{a}+3\mathbf{b})/4$ or $(3\mathbf{a}+\mathbf{b})/4]$	L26
(100)	**b**	**c**	**a**	$Pnnn$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L19
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L03
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa$ $(\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bmcm$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$ $(\mathbf{a}'/4)$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4)$	L24

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No. 135 $P4_2/mbc$ D_{4h}^{13}

$$\mathcal{G} = P\frac{4_2}{m}\frac{2_1}{b}\frac{2}{c}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/mbc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbam$	L44
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pcma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ma$	L28
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bbmb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmn$	L42
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmb$ $(\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24

No. 136 $P4_2/mnm$ D_{4h}^{14}

$$\mathcal{G} = P\frac{4_2}{m}\frac{2_1}{n}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/mnm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}mmm$	L47
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2_1m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L58
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pnmn$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmma$ $(\mathbf{a}'/4)$	L41
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23

No. 137 $P4_2/nmc$ D_{4h}^{15}

$$\mathcal{G} = P\frac{4_2}{n}\frac{2_1}{m}\frac{2}{c} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/nmc$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}m2$	L59
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $[(\mathbf{a}+\mathbf{b})/4]$	L46
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pmnm$ (origin 1) $(\mathbf{b}'/4)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$ $(\mathbf{b}'/4)$	L27
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/m11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L15
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{b}'/4)$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L39
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	or $Bbcb$ (or. 2) $[(\mathbf{a}'+\mathbf{b}')/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $(\mathbf{b}'/4)$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25

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No. 137 $P4_2/nmc$ D_{4h}^{15}

$$\mathcal{G} = P\frac{4_2}{n}\frac{2_1}{m}\frac{2}{c} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/nmc$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmn$	L46
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$ $[(\mathbf{a}+3\mathbf{b})/4$ or $(\mathbf{a}+3\mathbf{b})/4]$	L59
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$ $[(\mathbf{a}+\mathbf{b})/4]$	L23
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pmnm$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/m11$	L15
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2m$ $(\mathbf{a}'/4)$	L27
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{a}'+\mathbf{b}')/4]$ or $Bbcb$ (or. 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $(\mathbf{a}'/4)$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L25
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$Bbcb$ (or. 1) $[(\mathbf{b}'+\mathbf{d})/4]$ or $Bbcb$ (or. 2) $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban$ $(\mathbf{a}'/4)$	L39
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25

No. 138 $P4_2/ncm$ D_{4h}^{16}

$$\mathcal{G} = P\frac{4_2}{n}\frac{2_1}{c}\frac{2}{m} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/ncm$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}2_1m$	L58
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}mme$ $[(\mathbf{a}+3\mathbf{b})/4$ or $(3\mathbf{a}+\mathbf{b})/4]$	L48
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L26
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Pbnb$ $[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pb2b$ $(\mathbf{b}'/4)$	L30
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1/b11$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{b}'/4)$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Bmcm$ $[(\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L38
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$ $(\mathbf{b}'/4)$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{b}'/4)$	L24

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No. 138 $P4_2/ncm$ D_{4h}^{16}

$$\mathcal{G} = P\frac{4_2}{n}\frac{2_1}{c}\frac{2}{m} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$P4_2/ncm$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}mme$	L48
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2_1m$ $[(\mathbf{a}+3\mathbf{b})/4$ or $(3\mathbf{a}+\mathbf{b})/4]$	L58
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$ $[(\mathbf{a}+\mathbf{b})/4]$	L26
(100)	**b**	**c**	**a**	$Pbnb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pb2b$ $(\mathbf{a}'/4)$	L30
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Bmcm$ $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmam$ $(\mathbf{a}'/4)$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4)$	L24
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Bmcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa$ $(\mathbf{a}'/4)$	L38
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24

No. 139 $I4/mmm$ D_{4h}^{17}

$$\mathcal{G} = I\frac{4}{m}\frac{2}{m}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4/mmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/mmm$	L61
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/nmm$	L64
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4mm$	L55
(100)	**b**	**c**	**a**	$Immm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L46
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cmmm$	L47
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cmme$ $(\mathbf{b}'/4)$	L48
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cmm2$	L26

No. 140 $I4/mcm$ D_{4h}^{18}

$$\mathcal{G} = I\frac{4}{m}\frac{2}{c}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4/mcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/mbm$	L63
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/nbm$	L62
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4bm$	L56
(100)	**b**	**c**	**a**	$Icma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmb$	L38
(010)	$-\mathbf{a}$	**c**	**b**		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbma$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L45
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cmme$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L48
(1$\bar{1}$0)	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cmmm$ $(\mathbf{a}'/4)$	L47
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cmm2$ $(\mathbf{a}'/4)$	L26

No. 141 $I4_1/amd$ D_{4h}^{19}

$$\mathcal{G} = I\frac{4_1}{a}\frac{2}{m}\frac{2}{d} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_1/amd$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$	L59
						$p\bar{4}m2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L59
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$pmmb$ $(\mathbf{b}/4)$	L41
						$pmma$ $(\mathbf{a}/4)$	L41
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$ $(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pmm2$	L23
(100)	**b**	**c**	**a**	$Imcm$ $(\mathbf{a}'/4+\mathbf{b}'/8)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$ $(\mathbf{a}'/4+\mathbf{b}'/8)$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pman$ $(\mathbf{b}'/8)$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4+\mathbf{b}'/8)$	L24
(010)	$-\mathbf{a}$	**c**	**b**	$Imcm$ $(\mathbf{a}'/4+3\mathbf{b}'/8)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$ $(\mathbf{a}'/4+3\mathbf{b}'/8)$	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pman$ $(\mathbf{b}'/8)$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4+3\mathbf{b}'/8)$	L24
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fddd$ (or. 1) or $Fddd$ (or. 2) $[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/8]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$ $[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$	L22
						$c222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L22
						$\widehat{p}112/b$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L16
						$\widehat{p}112/a$ $[(3\mathbf{a}'+\mathbf{b}')/8$ or $(\mathbf{a}'+3\mathbf{b}')/8]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$ $(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$	L03
(1$\bar{1}$0)	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Fddd$ (or. 1) or $Fddd$ (or. 2) $[3(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/8]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$	L22
						$c222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L22
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}112/a$ $[(3\mathbf{a}'+\mathbf{b}')/8$ or $(\mathbf{a}'+3\mathbf{b}')/8]$	L16
						$\widehat{p}112/b$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L16
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$ $(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$	L03

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No. 141 $I4_1/amd$ D_{4h}^{19}

$\mathcal{G} = I\frac{4_1}{a}\frac{2}{m}\frac{2}{d}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_1/amd$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	*pmmb*	L41
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pmma* $[(\mathbf{a}+\mathbf{b})/4]$	L41
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}m2$ $(3\mathbf{b}/4)$	L59
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}m2$ $(\mathbf{b}/4)$	L59
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	*pmm2* $(\mathbf{b}/4)$	L23
(100)	**b**	**c**	**a**	*Imcm*	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pmam*	L40
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pman* $[(\mathbf{a}'+\mathbf{b}')/4]$	L42
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pma2*	L24
(010)	$-\mathbf{a}$	**c**	**b**	*Imcm* $[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	*pman*	L42
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	*pman* $[(\mathbf{a}'+\mathbf{b}')/4]$	L40
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	*pma2* $[(\mathbf{a}'+\mathbf{b}')/4]$	L24
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	*Fddd* (or. 1) $[(\mathbf{a}'+3\mathbf{b}'+\mathbf{d})/8]$ or *Fddd* (or. 2) $[(\mathbf{a}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/a$	L16
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/b$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L16
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[(\mathbf{a}'+3\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[(3\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$	$\widehat{p}112$ $[(\mathbf{a}'+3\mathbf{b}')/8$	
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	or $(3\mathbf{a}'+\mathbf{b}')/8]$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	*Fddd* (or. 1) $[(3\mathbf{a}'+\mathbf{b}'+\mathbf{d})/8]$ or *Fddd* (or. 2) $[(\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/a$	L16
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/b$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L16
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[(3\mathbf{a}'+\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[(\mathbf{a}'+3\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$	$\widehat{p}112$ $[(\mathbf{a}'+3\mathbf{b}')/4$	
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	or $(3\mathbf{a}'+\mathbf{b}')/8]$	L03

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 142, pp. 501–502.

No. 142 $I4_1/acd$ D_{4h}^{20}

$\mathcal{G} = I\frac{4_1}{a}\frac{2}{c}\frac{2}{d}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_1/acd$ (origin 1)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$	L60
						$p\bar{4}b2$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	L60
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$pbab$ ($\mathbf{b}/4$)	L43
						$pbaa$ ($\mathbf{a}/4$)	L43
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$ $(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$pba2$	L25
(100)	**b**	**c**	**a**	$Ibca$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ ($\mathbf{b}'/8$)	L43
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pba2$ ($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	L25
(010)	$-\mathbf{a}$	**c**	**b**	$Ibca$ ($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$ ($\mathbf{a}'/4 + 3\mathbf{b}'/8$)	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ ($\mathbf{b}'/8$)	L43
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pba2$ ($\mathbf{a}'/4 + \mathbf{b}'/8$)	L25
(110)	$(-\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}+\mathbf{b})$	$Fddd$ (or. 1) $[(\mathbf{a}' + \mathbf{d})/4]$ or $Fddd$ (or. 2) $[(3\mathbf{a}'+\mathbf{b}'+3\mathbf{d})/8]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ ($\mathbf{b}'/4$)	L22
						$c222$ ($\mathbf{a}'/4$)	L22
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}112/a$ $[(\mathbf{a}' + \mathbf{b}')/8]$	L16
						$\widehat{p}112/b$ $[(\mathbf{a}' + 3\mathbf{b}')/8$ or $(3\mathbf{a}' + \mathbf{b}')/8]$	L16
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d};$ $(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ ($\mathbf{a}'/4$ or $\mathbf{b}'/4$)	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	**c**	$(\mathbf{a}-\mathbf{b})$	$Fddd$ (or. 1) $(\mathbf{b}'/4)$ or $Fddd$ (or. 2) $[(\mathbf{a}' + 3\mathbf{b}' + \mathbf{d})/8]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ ($\mathbf{b}'/4$)	L22
						$c222$ ($\mathbf{a}'/4$)	L22
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$ $\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}112/b$ $[(\mathbf{a}'+3\mathbf{b}')/8]$	L16
						$\widehat{p}112/a$ $[(\mathbf{a}' + \mathbf{b}')/8]$	L16
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d};$ $(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ ($\mathbf{a}'/4$ or $\mathbf{b}'/4$)	L03

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No. 142 $I4_1/acd$ D_{4h}^{20}

$$\mathcal{G} = I\,^{4_1}_{a}\,^{2}_{c}\,^{2}_{d} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I4_1/acd$ (origin 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$pbab$	L43
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $[(\mathbf{a}+\mathbf{b})/4]$	L43
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}b2$ $(3\mathbf{b}/4)$	L60
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}b2$ $(\mathbf{b}/4)$	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pba2$ $(\mathbf{b}/4)$	L25
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$Ibca$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
(010)	$-\mathbf{a}$	$\mathbf{c}$	$\mathbf{b}$	$Ibca$ $[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbaa$	L43
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{a}'/4)$	L25
(110)	$(-\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})$	$Fddd$ (or. 1) $[3(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/8]$ or $Fddd$ (or. 2)	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/b$	L16
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/a$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L16
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[3(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L03
$(1\bar{1}0)$	$(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})$	$Fddd$ (or. 1) $[(\mathbf{a}'+\mathbf{b}'+3\mathbf{d})/8]$ or $Fddd$ (or. 2) $[(\mathbf{a}'+\mathbf{b}')/4]$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/b$	L16
					$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/a$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L16
					$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[3(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L03

Auxiliary tables for Laue class $D_{4h}-4/mmm$

Centring type P

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\bar{n}m0)$	$\mathbf{c}$	$m\mathbf{a}+n\mathbf{b}$	$-q\mathbf{a}+p\mathbf{b}$			
$(\bar{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(nm0)$	$\mathbf{c}$	$m\mathbf{a}-n\mathbf{b}$	$q\mathbf{a}+p\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\bar{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(m0n)$	$\mathbf{b}$	$m\mathbf{c}-n\mathbf{a}$	$q\mathbf{c}+p\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(m0\bar{n})$	$\mathbf{b}$	$m\mathbf{c}+n\mathbf{a}$	$-q\mathbf{c}+p\mathbf{a}$			
(hhl)	$\mathbf{a}-\mathbf{b}$	$n(\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$
$(\bar{h}\bar{h}l)$	$\mathbf{a}-\mathbf{b}$	$n(\mathbf{a}+\mathbf{b})+m\mathbf{c}$	$-p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$			
$(h\bar{h}l)$	$\mathbf{a}+\mathbf{b}$	$n(\mathbf{b}-\mathbf{a})-m\mathbf{c}$	$p(\mathbf{b}-\mathbf{a})+q\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$
$(\bar{h}hl)$	$\mathbf{a}+\mathbf{b}$	$n(\mathbf{b}-\mathbf{a})+m\mathbf{c}$	$-p(\mathbf{b}-\mathbf{a})+q\mathbf{c}$			
l odd $\Rightarrow n=l, m=2h$; l even $\Rightarrow n=l/2, m=h$						

Arithmetic class 422P

Serial No.	89	90	91	92	93	94	95	96
Group type	D_4^1	D_4^2	D_4^3	D_4^4	D_4^5	D_4^6	D_4^7	D_4^8
Group	$P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$	$P4_322$	$P4_32_12$
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112$	$P112$	$P112_1$	$P112_1$	$P112$	$P112$	$P112_1$	$P112_1$
$(0mn)$ $(0\overline{m}n)$	$P112$	$P112_1$ $(\mathbf{b}/4)$	$P112$ $(\mathbf{c}/4)$	$P112_1$ $(\mathbf{b}/4+3\mathbf{c}/8)$	$P112$	$P112_1$ $(\mathbf{b}+\mathbf{c})/4$	$P112$ $(\mathbf{c}/4)$	$P112_1$ $(\mathbf{b}/4+\mathbf{c}/8)$
$(m0n)$ $(m0\overline{n})$		$P112_1$ $(\mathbf{a}/4)$	$P112$	$P112_1$ $(\mathbf{a}/4+\mathbf{c}/8)$		$P112_1$ $(\mathbf{a}+\mathbf{c})/4$	$P112$	$P112_1$ $(\mathbf{a}/4+3\mathbf{c}/8)$
(hhl) $(\overline{h}\overline{h}l)$	$B112$	$B112$	$B112$ $(\mathbf{c}/8)$	$B112$ $(\mathbf{c}/4)$	$B112$ $(\mathbf{c}/4)$	$B112$	$B112$ $(3\mathbf{c}/8)$	$B112$ $(\mathbf{c}/4)$
$(h\overline{h}l)$ $(\overline{h}hl)$			$B112$ $(3\mathbf{c}/8)$	$B112$			$B112$ $(\mathbf{c}/8)$	$B112$

Arithmetic class 4$mm$$P$

Serial No.	99	100	101	102	103	104	105	106
Group type	C_{4v}^1	C_{4v}^2	C_{4v}^3	C_{4v}^4	C_{4v}^5	C_{4v}^6	C_{4v}^7	C_{4v}^8
Group	$P4mm$	$P4bm$	$P4_2cm$	$P4_2nm$	$P4cc$	$P4nc$	$P4_2mc$	$P4_2bc$
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$
$(0mn)$ $(0\overline{m}n)$	$P11m$	$P11a$ $(\mathbf{a}/4)$	$P11b$	$P11n$	$P11b$	$P11n$	$P11m$	$P11a$ $(\mathbf{a}/4)$
$(m0n)$ $(m0\overline{n})$		$P11b$ $(\mathbf{b}/4)$	$P11a$		$P11a$			$P11b$ $(\mathbf{b}/4)$
(hhl) $(\overline{h}\overline{h}l)$	$B11m$	$B11m$ $(\mathbf{a}-\mathbf{b})/4$	$B11m$	$B11m$	$B11b$	$B11b$ $(\mathbf{a}-\mathbf{b})/4$	$B11b$	$B11b$ $(\mathbf{a}-\mathbf{b})/4$
$(h\overline{h}l)$ $(\overline{h}hl)$		$B11m$ $(\mathbf{a}+\mathbf{b})/4$				$B11b$ $(\mathbf{a}+\mathbf{b})/4$		$B11b$ $(\mathbf{a}+\mathbf{b})/4$

Arithmetic classes $\overline{4}2m$$P$ and $\overline{4}m2$$P$

Serial No.	111	112	113	114	115	116	117	118
Group type	D_{2d}^1	D_{2d}^2	D_{2d}^3	D_{2d}^4	D_{2d}^5	D_{2d}^6	D_{2d}^7	D_{2d}^8
Group	$P\overline{4}2m$	$P\overline{4}2c$	$P\overline{4}2_1m$	$P\overline{4}2_1c$	$P\overline{4}m2$	$P\overline{4}c2$	$P\overline{4}b2$	$P\overline{4}n2$
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$	$P112$
$(0mn)$ $(0\overline{m}n)$	$P112$	$P112$ $(\mathbf{c}/4)$	$P112_1$ $(\mathbf{b}/4)$	$P112_1$ $(\mathbf{b}+\mathbf{c})/4$	$P11m$	$P11b$	$P11a$ $(\mathbf{a}/4)$	$P11n$ $(\mathbf{a}/4)$
$(m0n)$ $(m0\overline{n})$			$P112_1$ $(\mathbf{a}/4)$	$P112_1$ $(\mathbf{a}+\mathbf{c})/4$		$P11a$	$P11b$ $(\mathbf{b}/4)$	$P11n$ $(\mathbf{b}/4)$
(hhl) $(\overline{h}\overline{h}l)$	$B11m$	$B11b$	$B11m$ $(\mathbf{a}-\mathbf{b})/4$	$B11b$ $(\mathbf{a}-\mathbf{b})/4$	$B112$	$B112$ $(\mathbf{c}/4)$	$B112$ $(\mathbf{a}+\mathbf{b})/4$	$B112$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
$(h\overline{h}l)$ $(\overline{h}hl)$			$B11m$ $(\mathbf{a}+\mathbf{b})/4$	$B11b$ $(\mathbf{a}+\mathbf{b})/4$			$B112$ $(\mathbf{a}-\mathbf{b})/4$	$B112$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$

Arithmetic class $4/mmmP$

Serial No.	123	124	125		126	
Group type	D_{4h}^1	D_{4h}^2	D_{4h}^3		D_{4h}^4	
Group	$P4/mmm$	$P4/mcc$	$P4/mbm$		$P4/nnc$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}\overline{n}0)$ $(nm0)$	$P112/m$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b})/4$	$P112/n$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$P112/m$	$P112/b$	$P112/a$ $(\mathbf{a}+\mathbf{b})/4$	$P112/a$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
$(m0n)$ $(m0\overline{n})$		$P112/a$	$P112/b$ $(\mathbf{a}+\mathbf{b})/4$	$P112/b$		
(hhl) $(\overline{h}\overline{h}l)$	$B112/m$	$B112/b$	$B112/m$ $(\mathbf{a}-\mathbf{b})/4$	$B112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/b$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)
$(h\overline{h}l)$ $(\overline{h}hl)$			$B112/m$ $(\mathbf{a}+\mathbf{b})/4$	$B112/m$	$B112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$B112/b$

Serial No.	127	128	129		130	
Group type	D_{4h}^5	D_{4h}^6	D_{4h}^7		D_{4h}^8	
Group	$P4/mbm$	$P4/mnc$	$P4/nmm$		$P4/ncc$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112/m$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b})/4$	$P112/n$	$P112/n$ $(\mathbf{a}+\mathbf{b})/4$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$P112_1/a$	$P112_1/n$	$P112_1/m$ $(\mathbf{a}+\mathbf{b})/4$	$P112_1/m$	$P112_1/b$ $(\mathbf{a}+\mathbf{b})/4$	$P112_1/b$
$(m0n)$ $(m0\overline{n})$	$P112_1/b$				$P112_1/a$ $(\mathbf{a}+\mathbf{b})/4$	$P112_1/a$
(hhl) $(\overline{h}\overline{h}l)$	$B112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/m$ $(\mathbf{a}-\mathbf{b})/4$	$B112/m$	$B112/b$ $(\mathbf{a}-\mathbf{b})/4$	$B112/b$
$(h\overline{h}l)$ $(\overline{h}hl)$			$B112/m$ $(\mathbf{a}+\mathbf{b})/4$	$B112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/b$ $(\mathbf{a}+\mathbf{b})/4$	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)

Serial No.	131	132	133		134	
Group type	D_{4h}^9	D_{4h}^{10}	D_{4h}^{11}		D_{4h}^{12}	
Group	$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$		$P4_2/nnm$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112/m$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$P112/m$	$P112/b$	$P112/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/a$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
$(m0n)$ $(m0\overline{n})$		$P112/a$	$P112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/b$		
(hhl) $(\overline{h}\overline{h}l)$	$B112/b$	$B112/m$	$B112/b$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/m$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$	$B112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)
$(h\overline{h}l)$ $(\overline{h}hl)$			$B112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$B112/b$	$B112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$B112/m$

Arithmetic class $4/mmmP$ (*cont.*)

Serial No.	135	136	137		138	
Group type	D_{4h}^{13}	D_{4h}^{14}	D_{4h}^{15}		D_{4h}^{16}	
Group	$P4_2/mbc$	$P4_2/mnm$	$P4_2/nmc$		$P4_2/ncm$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$P112/m$	$P112/m$	$P112/n$	$P112/n$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
$(0mn)$ $(0\overline{m}n)$	$P112_1/a$	$P112_1/n$	$P112_1/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112_1/m$	$P112_1/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112_1/b$
$(m0n)$ $(m0\overline{n})$	$P112_1/b$				$P112_1/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112_1/a$
(hhl) $(\overline{h}hl)$	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/m$	$B112/b$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$	$B112/b$	$B112/m$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$	$B112/m$
$(h\overline{h}l)$ $(\overline{h}hl)$			$B112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$B112/b$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$B112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$B112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)

Centring type *I*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{n}m0)$	$\mathbf{c}$	$m\mathbf{a}+n\mathbf{b}$	$-q\mathbf{a}+p\mathbf{b}$			
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(nm0)$	$\mathbf{c}$	$m\mathbf{a}-n\mathbf{b}$	$q\mathbf{a}+p\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\overline{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(m0n)$	$\mathbf{b}$	$m\mathbf{c}-n\mathbf{a}$	$q\mathbf{c}+p\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(m0\overline{n})$	$\mathbf{b}$	$m\mathbf{c}+n\mathbf{a}$	$-q\mathbf{c}+p\mathbf{a}$			
(hhl)	$\mathbf{a}-\mathbf{b}$	$n\widehat{\mathbf{a}}-m\mathbf{c}$	$p\widehat{\mathbf{a}}+q\mathbf{c}$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$
$(\overline{h}hl)$	$\mathbf{a}-\mathbf{b}$	$n\widehat{\mathbf{a}}+m\mathbf{c}$	$-p\widehat{\mathbf{a}}+q\mathbf{c}$			
$(h\overline{h}l)$	$\mathbf{a}+\mathbf{b}$	$n\widehat{\mathbf{a}}-m\mathbf{c}$	$p\widehat{\mathbf{a}}+q\mathbf{c}$	$(\mathbf{b}-\mathbf{a}+\mathbf{c})/2$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$
$(\overline{h}hl)$	$\mathbf{a}+\mathbf{b}$	$n\widehat{\mathbf{a}}+m\mathbf{c}$	$-p\widehat{\mathbf{a}}+q\mathbf{c}$			
l odd $\Rightarrow n=2l, m=2h+l$; l even $\Rightarrow n=l, m=h+l/2$						

Arithmetic classes $422I$ and $4mmI$

Serial No.	97	98	107	108	109	110
Group type	D_4^9	D_4^{10}	C_{4v}^9	C_{4v}^{10}	C_{4v}^{11}	C_{4v}^{12}
Group	$I422$	$I4_122$	$I4mm$	$I4cm$	$I4_1md$	$I4_1cd$
$(mn0)$ $(\overline{n}m0)$ $(\overline{m}n0)$ $(nm0)$	$I112$	$I112$	$I112$	$I112$	$I112$	$I112$
$(0mn)$ $(0\overline{m}n)$	$I112$	$I112$ $(\mathbf{b}/4+\mathbf{c}/8)$	$I11m$	$I11b$	$I11m$	$I11b$
$(m0n)$ $(m0\overline{n})$		$I112$ $(\mathbf{a}/4+3\mathbf{c}/8)$		$I11a$		$I11a$
(hhl) $(\overline{h}hl)$	$A112$	$A112$	$A11m$	$A11m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$A11n$ $(\mathbf{a}-\mathbf{b})/8$	$A11n$ $3(\mathbf{a}-\mathbf{b})/8$
$(h\overline{h}l)$ $(\overline{h}hl)$					$A11n$ $3(\mathbf{a}+\mathbf{b})/8$	$A11n$ $(\mathbf{a}+\mathbf{b})/8$

Arithmetic classes $\overline{4}m2I$ and $\overline{4}2mI$

Serial No. Group type Group	119 D_{2d}^{9} $I\overline{4}m2$	120 D_{2d}^{10} $I\overline{4}c2$	121 D_{2d}^{11} $I\overline{4}2m$	122 D_{2d}^{12} $I\overline{4}2d$
$(mn0)$ $(\overline{m}n0)$ $(\overline{m}n0)$ $(nm0)$	$I112$	$I112$	$I112$	$I112$
$(0mn)$ $(0\overline{m}n)$	$I11m$	$I11b$	$I112$	$I112$ $(\mathbf{b}/4+\mathbf{c}/8)$
$(m0n)$ $(m0\overline{n})$		$I11a$		$I112$ $(\mathbf{a}/4+3\mathbf{c}/8)$
(hhl) $(\overline{h}\overline{h}l)$ $(h\overline{h}l)$ $(\overline{h}hl)$	$A112$	$A112$ $(\mathbf{c}/4)$	$A11m$	$A11n$ $(\mathbf{a}-\mathbf{b})/8$ $A11n$ $3(\mathbf{a}+\mathbf{b})/8$

Arithmetic class $4/mmmI$

Serial No. Group type Group	139 D_{4h}^{17} $I4/mmm$	140 D_{4h}^{18} $I4/mcm$	141 D_{4h}^{19} $I4_1/amd$		142 D_{4h}^{20} $I4_1acd$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(mn0)$ $(\overline{m}n0)$ $(\overline{m}n0)$ $(nm0)$	$A112/a$	$A112/a$	$I112/b$ $(\mathbf{b}+\mathbf{c})/8$	$I112/b$	$I112/b$ $(\mathbf{b}+\mathbf{c})/8$	$I112/b$
$(0mn)$ $(0\overline{m}n)$	$I112/m$	$I112/b$	$I112/m$ $(\mathbf{b}/4+\mathbf{c}/8)$	$I112/m$	$I112/b$ $(\mathbf{b}/4+\mathbf{c}/8)$	$I112/b$
$(m0n)$ $(m0\overline{n})$		$I112/a$	$I112/m$ $(\mathbf{a}/4+3\mathbf{c}/8)$	$I112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$I112/a$ $(\mathbf{a}/4+3\mathbf{c}/8)$	$I112/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
(hhl) $(\overline{h}\overline{h}l)$ $(h\overline{h}l)$ $(\overline{h}hl)$	$A112/m$	$A112/m$	$A112/a$ $3(\mathbf{a}/4+\mathbf{c}/8)$ $A112/a$ $(\mathbf{a}/4+\mathbf{c}/8)$	$A112/a$ $(\mathbf{a}-\mathbf{b}+\mathbf{c})/4$ $A112/a$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)	$A112/a$ $(\mathbf{a}/4+3\mathbf{c}/8)$ $A112/a$ $3(\mathbf{a}/4+\mathbf{c}/8)$	$A112/a$

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 143, p. 507.

Laue class $C_{3i} - \overline{3}$

Geometric class $C_3 - 3$

No. 143 $P3$ C_3^1

$$\mathcal{G} = P3$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P3$	$s\mathbf{d}$	$p3$ L65

No. 144 $P3_1$ C_3^2

$$\mathcal{G} = P3_1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P3_1$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p1$ L01

No. 145 $P3_2$ C_3^3

$$\mathcal{G} = P3_2$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P3_2$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p1$ L01

No. 146 $R3$ C_3^4

$$\mathcal{G} = R3$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	**a**	**b**	**c**	$R3$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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Geometric class $C_{3i} - \overline{3}$

No. 147 $P\overline{3}$ C_{3i}^1

$$\mathcal{G} = P\overline{3}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P\overline{3}$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p\overline{3}$ L66

No. 148 $R\overline{3}$ C_{3i}^2

$$\mathcal{G} = R\overline{3}$$

Orientation orbit: HEXAG. AXES $(hkil)$	Orientation orbit: RHOMB. AXES (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	(111)	**a** **b** **c**	$R\overline{3}$	$[0\mathbf{d}, \ [\frac{1}{2}\mathbf{d},$	$p\overline{3}$ L66
				$\frac{1}{3}\mathbf{d}, \ \| \ \frac{5}{6}\mathbf{d},$	$p\overline{3}\ [(2\mathbf{a}+\mathbf{b})/3]$ L66
				$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\overline{3}\ [(\mathbf{a}+2\mathbf{b})/3]$ L66
				$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$ L65

Laue class $D_{3d} - \overline{3}m$

Geometric class $D_3 - 32$

No. 149 $P312$ D_3^1

$$\mathcal{G} = P312$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P312$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p312$ L67
			$[s\mathbf{d}, -s\mathbf{d}]$	$p3$ L65
$(01\overline{1}0)$	**c** **a** $\mathbf{a}+2\mathbf{b}$	$A112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$ L03
$(\overline{1}010)$	**c** **b** $-(2\mathbf{a}+\mathbf{b})$			
$(1\overline{1}00)$	**c** $-(\mathbf{a}+\mathbf{b})$ $(\mathbf{a}-\mathbf{b})$			
$(\overline{1}2\overline{1}0)$	**c** $2\mathbf{a}+\mathbf{b}$ **b**	$A121$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$ L08
$(\overline{1}\overline{1}20)$	**c** $(\mathbf{b}-\mathbf{a})$ $-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$ L09
$(2\overline{1}\overline{1}0)$	**c** $-(\mathbf{a}+2\mathbf{b})$ **a**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$ L01

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No. 150 $P321$ D_3^2

$$\mathcal{G} = P321$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P321$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p321$	L68
					$[s\mathbf{d}, -s\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A121$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$				
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$				

No. 151 $P3_112$ D_3^3

$$\mathcal{G} = P3_112$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3_112$	$[0\mathbf{d}, [\frac{1}{2}\mathbf{d},$	$\widehat{c}_2121$	L10
					$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$\widehat{c}_3121$	L10
					$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$\widehat{c}_1121$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p1$	L01
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A112$ $(\mathbf{a}'/6)$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/6)$	L03
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A112$ $(\mathbf{a}'/3)$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/3)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A121$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A121$ $(\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$ $(\mathbf{a}'/3)$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$ $(\mathbf{a}'/3)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A121$ $(\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p121$ $(\mathbf{a}'/6)$	L08
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$ $(\mathbf{a}'/6)$	L09
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 152 $P3_121$ D_3^4

$$\mathcal{G} = P3_121$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3_121$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$	$\widehat{c}_3211$	L10
					$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$\widehat{c}_1211$	L10
					$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$\widehat{c}_2211$	L10
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p1$	L01
$(01\overline{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A121\ (\mathbf{a}'/3)$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121\ (\mathbf{a}'/3)$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11\ (\mathbf{a}'/3)$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\overline{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A121\ (\mathbf{a}'/6)$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121\ (\mathbf{a}'/6)$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11\ (\mathbf{a}'/6)$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(1\overline{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A121$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\overline{1}2\overline{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A112\ (\mathbf{a}'/6)$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/6)$	L03
$(\overline{1}\overline{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A112$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(2\overline{1}\overline{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A112\ (\mathbf{a}'/3)$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/3)$	L03

No. 153 $P3_212$ D_3^5

$$\mathcal{G} = P3_212$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3_212$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$	$\widehat{c}_2121$	L10
					$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$\widehat{c}_1121$	L10
					$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$\widehat{c}_3121$	L10
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p1$	L01
$(01\overline{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A112\ (\mathbf{a}'/3)$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/3)$	L03
$(\overline{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A112$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(1\overline{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A112\ (\mathbf{a}'/6)$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/6)$	L03
$(\overline{1}2\overline{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A121$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\overline{1}\overline{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A121\ (\mathbf{a}'/6)$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121\ (\mathbf{a}'/6)$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11\ (\mathbf{a}'/6)$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(2\overline{1}\overline{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A121\ (\mathbf{a}'/3)$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p121\ (\mathbf{a}'/3)$	L08
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p12_11\ (\mathbf{a}'/3)$	L09
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 154 $P3_221$ D_3^6

$$\mathcal{G} = P3_221$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3_221$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$ $\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$ $\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$ $(\pm s+\frac{2}{3})\mathbf{d}]$	$\widehat{c}_3211$ $\widehat{c}_2211$ $\widehat{c}_1211$ $p1$	L10 L10 L10 L01
$(01\overline{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A121\ (\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p121\ (\mathbf{a}'/6)$ $p12_11\ (\mathbf{a}'/6)$ $p1$	L08 L09 L01
$(\overline{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A121\ (\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p121\ (\mathbf{a}'/3)$ $p12_11\ (\mathbf{a}'/3)$ $p1$	L08 L09 L01
$(1\overline{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A121$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p121$ $p12_11$ $p1$	L08 L09 L01
$(\overline{1}2\overline{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A112\ (\mathbf{a}'/3)$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/3)$	L03
$(\overline{1}\overline{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(2\overline{1}\overline{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A112\ (\mathbf{a}'/6)$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/6)$	L03

No. 155 $R32$ D_3^7

$$\mathcal{G} = R32$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$R32$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$ $\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$ $\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p321$ $p321\ [(2\mathbf{a}+\mathbf{b})/3]$ $p321\ [(\mathbf{a}+2\mathbf{b})/3]$ $p3$	L68 L68 L68 L65
$(01\overline{1}0)$	$(11\overline{1})$	$\mathbf{c}$	$\mathbf{a}$	$-\mathbf{c}_r$	$I121$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p121$ $p12_11\ (\mathbf{a}'/4)$ $p1$	L08 L09 L01
$(\overline{1}010)$	$(\overline{1}11)$	$\mathbf{c}$	$\mathbf{b}$	$-\mathbf{a}_r$				
$(1\overline{1}00)$	$(1\overline{1}1)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$-\mathbf{b}_r$				
$(\overline{1}2\overline{1}0)$	$(01\overline{1})$	$\mathbf{c}$	$\mathbf{a}_r$	$\mathbf{b}$	$I112$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\overline{1}\overline{1}20)$	$(\overline{1}01)$	$\mathbf{c}$	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$				
$(2\overline{1}\overline{1}0)$	$(1\overline{1}0)$	$\mathbf{c}$	$\mathbf{c}_r$	$\mathbf{a}$				

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Geometric class $C_{3v}-3m$

No. 156 $P3m1$ C_{3v}^1

$$\mathcal{G} = P3m1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3m1$	$s\mathbf{d}$	$p3m1$	L69
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A1m1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$				
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$				
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A11m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 157 $P31m$ C_{3v}^2

$$\mathcal{G} = P31m$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P31m$	$s\mathbf{d}$	$p31m$	L70
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A11m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11m$	L04
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11b$	L05
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A1m1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$				
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$				

No. 158 $P3c1$ C_{3v}^3

$$\mathcal{G} = P3c1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P3c1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A1a1$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$				
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$				
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A11a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p11a$	L05
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p11n$	L05
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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No. 159 $P31c$ C_{3v}^4

$$\mathcal{G} = P31c$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P31c$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A11a$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p11a$	L05
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p11n$	L05
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A1a1$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$				
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$				

No. 160 $R3m$ C_{3v}^5

$$\mathcal{G} = R3m$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$R3m$	$[s\mathbf{d},\ (s+\frac{1}{3})\mathbf{d},\ (s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$(11\bar{1})$	$\mathbf{c}$	$\mathbf{a}$	$-\mathbf{c}_r$	$I1m1$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}010)$	$(\bar{1}11)$	$\mathbf{c}$	$\mathbf{b}$	$-\mathbf{a}_r$				
$(1\bar{1}00)$	$(1\bar{1}1)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$-\mathbf{b}_r$				
$(\bar{1}2\bar{1}0)$	$(01\bar{1})$	$\mathbf{c}$	$\mathbf{a}_r$	$\mathbf{b}$	$I11m$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p11m$	L04
$(\bar{1}\bar{1}20)$	$(\bar{1}01)$	$\mathbf{c}$	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p11n$	L05
$(2\bar{1}\bar{1}0)$	$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{c}_r$	$\mathbf{a}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 161 $R3c$ C_{3v}^6

$$\mathcal{G} = R3c$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$R3c$	$[s\mathbf{d},\ (s+\frac{1}{6})\mathbf{d},$ $(s+\frac{1}{3})\mathbf{d},\ (s+\frac{1}{2})\mathbf{d},$ $(s+\frac{2}{3})\mathbf{d},\ (s+\frac{5}{6})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$(11\bar{1})$	$\mathbf{c}$	$\mathbf{a}$	$-\mathbf{c}_r$	$I1a1$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}010)$	$(\bar{1}11)$	$\mathbf{c}$	$\mathbf{b}$	$-\mathbf{a}_r$				
$(1\bar{1}00)$	$(1\bar{1}1)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$-\mathbf{b}_r$				
$(\bar{1}2\bar{1}0)$	$(01\bar{1})$	$\mathbf{c}$	$\mathbf{a}_r$	$\mathbf{b}$	$I11a$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p11a$	L05
$(\bar{1}\bar{1}20)$	$(\bar{1}01)$	$\mathbf{c}$	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p11b$	L05
$(2\bar{1}\bar{1}0)$	$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{c}_r$	$\mathbf{a}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1$	L01

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Geometric class $D_{3d} - \bar{3}m$

No. 162 $P\bar{3}1m$ D^1_{3d}

$$\mathcal{G} = P\bar{3}1\tfrac{2}{m}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{3}1m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{3}1m$	L71
					$[s\mathbf{d}, -s\mathbf{d}]$	$p31m$	L70
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $(\mathbf{b}'/4)$	L07
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A12/m1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/m1$ $(\mathbf{b}'/4)$	L15
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11

No. 163 $P\bar{3}1c$ D^2_{3d}

$$\mathcal{G} = P\bar{3}1\tfrac{2}{c}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{3}1c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{3}$	L66
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p312$	L67
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A112/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $(\mathbf{b}'/4)$	L07
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A12/a1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/a1$	L16
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/a1$ $(\mathbf{b}'/4)$	L17
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12

No. 164 $P\bar{3}m1$ D^3_{3d}

$$\mathcal{G} = P\bar{3}\tfrac{2}{m}1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{3}m1$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{3}m1$	L72
					$[s\mathbf{d}, -s\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A12/m1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/m1$ $(\mathbf{b}'/4)$	L15
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $(\mathbf{b}'/4)$	L07
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 165 $P\bar{3}c1$ D_{3d}^4

$$\mathcal{G} = P\bar{3}\tfrac{2}{c}1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	**a**	**b**	**c**	$P\bar{3}c1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{3}$	L66
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p321$	L68
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	**c**	**a**	$\mathbf{a}+2\mathbf{b}$	$A12/a1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/a1$	L16
$(\bar{1}010)$	**c**	**b**	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/a1$ $(\mathbf{b}'/4)$	L17
$(1\bar{1}00)$	**c**	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}2\bar{1}0)$	**c**	$2\mathbf{a}+\mathbf{b}$	**b**	$A112/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
$(\bar{1}\bar{1}20)$	**c**	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $(\mathbf{b}'/4)$	L07
$(2\bar{1}\bar{1}0)$	**c**	$-(\mathbf{a}+2\mathbf{b})$	**a**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03

No. 166 $R\bar{3}m$ D_{3d}^5

$$\mathcal{G} = R\bar{3}\tfrac{2}{m}$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	**a**	**b**	**c**	$R\bar{3}m$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
						$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}+\mathbf{b})/3]$	L72
						$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}+2\mathbf{b})/3]$	L72
						$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$		
						$(\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$(11\bar{1})$	**c**	**a**	$-\mathbf{c}_r$	$I12/m1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/m1$	L14
$(\bar{1}010)$	$(\bar{1}11)$	**c**	**b**	$-\mathbf{a}_r$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/m1$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L15
$(1\bar{1}00)$	$(1\bar{1}1)$	**c**	$-(\mathbf{a}+\mathbf{b})$	$-\mathbf{b}_r$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}2\bar{1}0)$	$(01\bar{1})$	**c**	$\mathbf{a}_r$	**b**	$I112/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/m$	L06
$(\bar{1}\bar{1}20)$	$(\bar{1}01)$	**c**	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L07
$(2\bar{1}\bar{1}0)$	$(1\bar{1}0)$	**c**	$\mathbf{c}_r$	**a**		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 167 $R\overline{3}c$ D^6_{3d}

$$\mathcal{G} = R\overline{3}\tfrac{2}{c}$$

Orientation orbit		Conventional basis of the scanning group			Scanning group	Linear orbit	Sectional layer group	
HEXAG. AXES ($hkil$)	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\mathcal{H}$	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	
(0001)	(111)	**a**	**b**	**c**	$R\overline{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$ $\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$ $\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$ $\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$ $\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$ $[\pm s\mathbf{d}, (\pm s + \frac{1}{6})\mathbf{d},$ $(\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d},$ $(\pm s + \frac{2}{3})\mathbf{d}, (\pm s + \frac{5}{6})\mathbf{d}]$	$p\overline{3}$ $p\overline{3}\ [(2\mathbf{a}+\mathbf{b})/3]$ $p\overline{3}\ [(\mathbf{a}+2\mathbf{b})/3]$ $p321$ $p321\ [(2\mathbf{a}+\mathbf{b})/3]$ $p321\ [(\mathbf{a}+2\mathbf{b})/3]$ $p3$	L66 L66 L66 L68 L68 L68 L65
$(01\overline{1}0)$	$(11\overline{1})$	**c**	**a**	$-\mathbf{c}_r$	$I12_1/a1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p12/a1$	L16
$(\overline{1}010)$	$(\overline{1}11)$	**c**	**b**	$-\mathbf{a}_r$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_1/a1$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L17
$(1\overline{1}00)$	$(1\overline{1}1)$	**c**	$-(\mathbf{a}+\mathbf{b})$	$-\mathbf{b}_r$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\overline{1}2\overline{1}0)$	$(01\overline{1})$	**c**	$\mathbf{a}_r$	**b**	$I112/a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/a$	L07
$(\overline{1}\overline{1}20)$	$(\overline{1}01)$	**c**	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/b$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L07
$(2\overline{1}\overline{1}0)$	$(1\overline{1}0)$	**c**	$\mathbf{c}_r$	**a**		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/4)$	L03

Auxiliary tables for Laue class $D_{3d} - \overline{3}m$

Centring type *P*

Arithmetic classes $312P$, $31mP$ and $\overline{3}1mP$

Orientation orbit	Conventional basis of the scanning group			Auxiliary basis of the scanning group		
($hkil$)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(\overline{h}2h\overline{h}l)$	$2\mathbf{a}+\mathbf{b}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	**b**	**c**	$2\mathbf{a}+\mathbf{b}$
$(\overline{hh}2hl)$	$\mathbf{b}-\mathbf{a}$	$-n(\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$-p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	**c**	$\mathbf{b}-\mathbf{a}$
$(2h\overline{hh}l)$	$-(\mathbf{a}+2\mathbf{b})$	$n\mathbf{a}-m\mathbf{c}$	$p\mathbf{a}+q\mathbf{c}$	**a**	**c**	$-\mathbf{a}+2\mathbf{b}$
l odd $\Rightarrow n = l, m = 2h$; l even $\Rightarrow n = l/2, m = h$						

Arithmetic classes $312P$, $31mP$ and $\overline{3}1mP$

Serial No.	149	151	153	157	159	162	163
Group type	D^1_3	D^3_3	D^5_3	C^2_{3v}	C^4_{3v}	D^1_{3d}	D^2_{3d}
Group	$P312$	$P3_112$	$P3_212$	$P31m$	$P31c$	$P\overline{3}1m$	$P\overline{3}1c$
$(\overline{h}2h\overline{h}l)$	$B112$	$B112$	$B112$	$B11m$	$B11b$	$B112/m$	$B112/b$
$(\overline{hh}2hl)$		$B112\ (\mathbf{c}/3)$	$B112\ (\mathbf{c}/6)$				
$(2h\overline{hh}l)$		$B112\ (\mathbf{c}/6)$	$B112\ (\mathbf{c}/3)$				

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Arithmetic classes $321P$, $3m1P$ and $\overline{3}m1P$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(0h\bar{h}l)$	$\mathbf{a}$	$n(\mathbf{a}+2\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}+2\mathbf{b})+q\mathbf{c}$	$\mathbf{a}+2\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(\bar{h}0hl)$	$\mathbf{b}$	$-n(2\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$-p(2\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$-(2\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$\mathbf{b}$
$(h\bar{h}0l)$	$-(\mathbf{a}+\mathbf{b})$	$n(\mathbf{a}-\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}-\mathbf{b})+q\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$
l odd $\Rightarrow n=l, m=2h$; l even $\Rightarrow n=l/2, m=h$						

Arithmetic classes $321P$, $3m1P$ and $\overline{3}m1P$

Serial No.	150	152	154	156	158	164	165
Group type	D_3^2	D_3^4	D_3^6	C_{3v}^1	C_{3v}^2	D_{3d}^3	D_{3d}^4
Group	$P321$	$P3_121$	$P3_221$	$P3m1$	$P3c1$	$P\bar{3}m1$	$P\bar{3}c1$
$(0h\bar{h}l)$	$B112$	$B112$ $(\mathbf{c}/3)$	$B112$ $(\mathbf{c}/6)$	$B11m$	$B11b$	$B112/m$	$B112/b$
$(\bar{h}0hl)$		$B112$ $(\mathbf{c}/6)$	$B112$ $(\mathbf{c}/3)$				
$(h\bar{h}0l)$		$B112$	$B112$				

Centring type *R*

Arithmetic classes $32R$, $3mR$ and $\overline{3}mR$

Orientation orbit		Conventional basis of the scanning group			Auxiliary basis of the scanning group		
HEXAG. AXES $(hkil)$	RHOMB. AXES (hkl)	$\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	$\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(0h\bar{h}l)$	(hhl)	$\mathbf{a}$	$n\mathbf{c}-m\mathbf{c}_r$	$p\mathbf{c}+q\mathbf{c}_r$	$\mathbf{c}$	$\mathbf{c}_r$	$\mathbf{a}$
$(\bar{h}0hl)$	(lhh)	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}_r$	$p\mathbf{c}+q\mathbf{a}_r$	$\mathbf{c}$	$\mathbf{a}_r$	$\mathbf{b}$
$(h\bar{h}0l)$	(hlh)	$-(\mathbf{a}+\mathbf{b})$	$n\mathbf{c}-m\mathbf{b}_r$	$p\mathbf{c}+q\mathbf{b}_r$	$\mathbf{c}$	$\mathbf{b}_r$	$-(\mathbf{a}+\mathbf{b})$
Transformation of indices from hexagonal to auxiliary monoclinic basis l odd $\Rightarrow n=l-2h, m=6h$; l even $\Rightarrow n=l/2-h, m=3h$							
Transformation of indices from rhombohedral to auxiliary monoclinic basis l odd $\Rightarrow n=l, m=2h+l$; l even $\Rightarrow n=l/2, m=h+l/2$							

Arithmetic classes $32R$, $3mR$ and $\overline{3}mR$

Serial No.		155	160	161	166	167
Group type		D_3^7	C_{3v}^5	C_{3v}^6	D_{3d}^5	D_{3d}^6
Group		$R32$	$R3m$	$R3c$	$R\bar{3}m$	$R\bar{3}c$
HEXAG. AXES	RHOMB. AXES					
$(0h\bar{h}l)$	(hhl)	$I112$	$I11m$	$I11a$	$I112/m$	$I112/a$
$(\bar{h}0hl)$	(lhh)					
$(h\bar{h}0l)$	(hlh)					

Laue class C_{6h} – $6/m$

Geometric class C_6 – 6

No. 168 $P6$ C_6^1

$$\mathcal{G} = P6$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6$	$s\mathbf{d}$	$p6$ L73

No. 169 $P6_1$ C_6^2

$$\mathcal{G} = P6_1$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6_1$	$[s\mathbf{d}, (s+\frac{1}{6})\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}, (s+\frac{5}{6})\mathbf{d}]$	$p1$ L01

No. 170 $P6_5$ C_6^3

$$\mathcal{G} = P6_5$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6_5$	$[s\mathbf{d}, (s+\frac{1}{6})\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{1}{2})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}, (s+\frac{5}{6})\mathbf{d}]$	$p1$ L01

No. 171 $P6_2$ C_6^4

$$\mathcal{G} = P6_2$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6_2$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p112$ L03

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No. 172 $P6_4$ C_6^5

$$\mathcal{G} = P6_4$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6_4$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p112$ L03

No. 173 $P6_3$ C_6^6

$$\mathcal{G} = P6_3$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6_3$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p3$ L65

Geometric class C_{3h} – $\overline{6}$

No. 174 $P\overline{6}$ C_{3h}^1

$$\mathcal{G} = P\overline{6}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P\overline{6}$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\overline{6}$ L74
			$[s\mathbf{d}, -s\mathbf{d}]$	$p3$ L65

Geometric class C_{6h} – $6/m$

No. 175 $P6/m$ C_{6h}^1

$$\mathcal{G} = P6/m$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P6/m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p6/m$ L75
			$[s\mathbf{d}, -s\mathbf{d}]$	$p6$ L73

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No. 176 $P6_3/m$ C_{6h}^2

$$\mathcal{G} = P6_3/m$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_3/m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\overline{3}$	L66
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\overline{6}$	L74
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65

Auxiliary tables for Laue class $C_{6h}-6/m$

Centring type P

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn\overline{m+n}0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m+n}mn0)$	$\mathbf{c}$	$m\mathbf{a}+(m+n)\mathbf{b}$	$-q\mathbf{a}+(p-q)\mathbf{b}$	$\mathbf{b}$	$-(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$
$(n\overline{m+n}m0)$	$\mathbf{c}$	$-(m+n)\mathbf{a}-n\mathbf{b}$	$(q-p)\mathbf{a}-p\mathbf{b}$	$-(\mathbf{a}+\mathbf{b})$	$\mathbf{a}$	$\mathbf{c}$

Arithmetic classes $6P$, $\overline{6}P$ and $6/mP$

Serial No.	168	169	170	171	172	173	174	175	176
Group type	C_6^1	C_6^2	C_6^3	C_6^4	C_6^5	C_6^6	C_{3h}^1	C_{6h}^1	C_{6h}^2
Group	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$	$P\overline{6}$	$P6/m$	$P6_3/m$
$(mn\overline{m+n}0)$ $(\overline{m+n}mn0)$ $(n\overline{m+n}m0)$	$P112$	$P112_1$	$P112_1$	$P112$	$P112$	$P112_1$	$P11m$	$P112/m$	$P112_1/m$

Laue class $D_{6h}-6/mmm$

Geometric class D_6 – 622

No. 177 $P622$ D_6^1

$$\mathcal{G} = P622$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P622$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p622$	L76
					$[s\mathbf{d}, -s\mathbf{d}]$	$p6$	L73
$(01\overline{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(\overline{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
$(1\overline{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\overline{1}2\overline{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(\overline{1}\overline{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
$(2\overline{1}\overline{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 178 $P6_122$ D_6^2

$$\mathcal{G} = P6_122$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{c}_1211$	L10
					$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$\widehat{c}_2211$	L10
					$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$\widehat{c}_3211$	L10
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$\widehat{c}_1121$	L10
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$\widehat{c}_2121$	L10
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$\widehat{c}_3121$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p1$	L01
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/4)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/4)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A2_122$ $(\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(7\mathbf{a}'/12)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(7\mathbf{a}'/12)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(7\mathbf{a}'/12)$	L03
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A2_122$ $(\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(5\mathbf{a}'/12)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(5\mathbf{a}'/12)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(5\mathbf{a}'/12)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2_122$ $(\mathbf{a}'/12)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/3)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/3)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/3)$	L03
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A2_122$ $(5\mathbf{a}'/12)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/6)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/6)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/6)$	L03
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A2_122$ $(\mathbf{a}'/4)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 179 $P6_522$ D_6^3

$\mathcal{G} = P6_522$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_522$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{c}_1211$	L10
					$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$\widehat{c}_3211$	L10
					$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$\widehat{c}_2211$	L10
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$\widehat{c}_1121$	L10
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$\widehat{c}_3121$	L10
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$\widehat{c}_2121$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p1$	L01
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/4)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/4)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A2_122$ $(\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(5\mathbf{a}'/12)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(5\mathbf{a}'/12)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(5\mathbf{a}'/12)$	L03
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A2_122$ $(\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(7\mathbf{a}'/12)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(7\mathbf{a}'/12)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(7\mathbf{a}'/12)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2_122$ $(5\mathbf{a}'/12)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/6)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/6)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/6)$	L03
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A2_122$ $(\mathbf{a}'/12)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/3)$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/3)$	L21
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/3)$	L03
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A2_122$ $(\mathbf{a}'/4)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$	L20
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 180 $P6_222$ D_6^4

$$\mathcal{G} = P6_222$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_222$	$[0\mathbf{d},\ [\frac{1}{2}\mathbf{d},$	$\widehat{c}_1222$	L10
					$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$\widehat{c}_3222$	L10
					$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$\widehat{c}_2222$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p112$	L03
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A222\ (\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222\ (\mathbf{a}'/6)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{a}'/6)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/6)$	L03
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A222\ (\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222\ (\mathbf{a}'/3)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{a}'/3)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/3)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A222\ (\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222\ (\mathbf{a}'/6)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{a}'/6)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/6)$	L03
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A222\ (\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222\ (\mathbf{a}'/3)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{a}'/3)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{a}'/3)$	L03
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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No. 181 $P6_422$ D_6^5

$$\mathcal{G} = P6_422$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_422$	$[0\mathbf{d},$ $[\frac{1}{2}\mathbf{d},$	$\widehat{c}_1222$	L10
					$\frac{1}{3}\mathbf{d},$ $\parallel$ $\frac{5}{6}\mathbf{d},$	$\widehat{c}_2222$	L10
					$\frac{2}{3}\mathbf{d}]$ $\frac{1}{6}\mathbf{d}]$	$\widehat{c}_3222$	L10
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p112$	L03
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$	$A222$ $(\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{a}'/3)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{a}'/3)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/3)$	L03
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$	$A222$ $(\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{a}'/6)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{a}'/6)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/6)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A222$ $(\mathbf{a}'/3)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{a}'/3)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{a}'/3)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/3)$	L03
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$	$A222$ $(\mathbf{a}'/6)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$ $(\mathbf{a}'/6)$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{a}'/6)$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/6)$	L03
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

No. 182 $P6_322$ D_6^6

$$\mathcal{G} = P6_322$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_322$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p321$	L68
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p312$	L67
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$ $(\mathbf{a}'/4)$	L20
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$ $(\mathbf{a}'/4)$	L21
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $(\mathbf{a}'/4)$	L03
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2_122$ $(\mathbf{a}'/4)$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122$	L20
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03

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Geometric class C_{6v} – 6*mm*

No. 183 *P*6*mm* C_{6v}^1

$\mathcal{G} = P6mm$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6mm$	$s\mathbf{d}$	$p6mm$	L77
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2mb$ $(\mathbf{b}'/4)$	L31
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2mb$ $(\mathbf{b}'/4)$	L31
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11

No. 184 *P*6*cc* C_{6v}^2

$\mathcal{G} = P6cc$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6cc$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p6$	L73
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2aa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2aa$	L30
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2an$ $(\mathbf{b}'/4)$	L34
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2aa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2aa$	L30
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2an$ $(\mathbf{b}'/4)$	L34
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12

No. 185 *P*6$_3$*cm* C_{6v}^3

$\mathcal{G} = P6_3cm$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_3cm$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$p31m$	L70
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2_1am$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1am$	L29
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ab$ $(\mathbf{b}'/4)$	L33
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2_1ma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_1ma$	L28
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11

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No. 186 $P6_3mc$ C_{6v}^4

$$\mathcal{G} = P6_3mc$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_3mc$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$A2_1ma$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2_1ma$	L28
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$A2_1am$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2_1am$	L29
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2_1ab\ (\mathbf{b}'/4)$	L33
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p1a1$	L12

Geometric class $D_{3h} - \bar{6}m2$ and $\bar{6}2m$

No. 187 $P\bar{6}m2$ D_{3h}^1

$$\mathcal{G} = P\bar{6}m2$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{6}m2$	$0\mathbf{d},\ \frac{1}{2}\mathbf{d}$	$p\bar{6}m2$	L78
					$[s\mathbf{d},\ -s\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Amm2$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$				
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$				
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Am2m$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pm2_1b$	L28
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11

No. 188 $P\bar{6}c2$ D_{3h}^2

$$\mathcal{G} = P\bar{6}c2$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{6}c2$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p312$	L67
					$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p\bar{6}$	L74
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Ama2$	$[s\mathbf{d},\ (s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$				
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$				
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Am2a$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$pm2a$	L31
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pm2_1n\ (\mathbf{a}'/4)$	L32
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11\ (\mathbf{a}'/4)$	L11

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No. 189 $P\bar{6}2m$ D_{3h}^3

$$\mathcal{G} = P\bar{6}2m$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{6}2m$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{6}2m$	L79
					$[s\mathbf{d}, -s\mathbf{d}]$	$p31m$	L70
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Am2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2m$	L27
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1b$	L28
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$	L11
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Amm2$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$				
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$				

No. 190 $P\bar{6}2c$ D_{3h}^4

$$\mathcal{G} = P\bar{6}2c$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{6}2c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p321$	L68
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{6}$	L74
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3$	L65
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Am2a$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pm2a$	L31
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pm2_1n$ $(\mathbf{a}'/4)$	L32
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pm11$ $(\mathbf{a}'/4)$	L11
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Ama2$	$[s\mathbf{d}, (s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$				
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$				

Geometric class $D_{6h}-6/mmm$

No. 191 $P6/mmm$ D_{6h}^1

$$\mathcal{G} = P6\frac{6}{m}\frac{2}{m}\frac{2}{m}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6/mmm$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p6/mmm$	L80
					$[s\mathbf{d}, -s\mathbf{d}]$	$p6mm$	L77
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Ammm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmb$ $(\mathbf{b}'/4)$	L41
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Ammm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmb$ $(\mathbf{b}'/4)$	L41
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23

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No. 192 $P6/mcc$ D^2_{6h}

$$\mathcal{G} = P6\frac{6}{m}\frac{2}{c}\frac{2}{c}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6/mcc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p6/m$	L75
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p622$	L76
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p6$	L73
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Amaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pman$ $(\mathbf{b}'/4)$	L42
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4)$	L24
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Amaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pman$ $(\mathbf{b}'/4)$	L42
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ $(\mathbf{a}'/4)$	L24

No. 193 $P6_3/mcm$ D^3_{6h}

$$\mathcal{G} = P\frac{6_3}{m}\frac{2}{c}\frac{2}{m}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_3/mcm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{3}1m$	L71
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{6}2m$	L79
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p31m$	L70
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Amam$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmab$ $(\mathbf{b}'/4)$	L45
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Amma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmma$	L41
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $(\mathbf{b}'/4)$	L46
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$ $(\mathbf{a}'/4)$	L23

No. 194 $P6_3/mmc$ D^4_{6h}

$$\mathcal{G} = P\frac{6_3}{m}\frac{2}{m}\frac{2}{c}$$

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P6_3/mmc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{3}m1$	L72
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{6}m2$	L78
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p3m1$	L69
$(01\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{a}+2\mathbf{b}$	$Amma$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmma$	L41
$(\bar{1}010)$	$\mathbf{c}$	$\mathbf{b}$	$-(2\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $(\mathbf{b}'/4)$	L46
$(1\bar{1}00)$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$(\mathbf{a}-\mathbf{b})$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$ $(\mathbf{a}'/4)$	L23
$(\bar{1}2\bar{1}0)$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$	$\mathbf{b}$	$Amam$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmam$	L40
$(\bar{1}\bar{1}20)$	$\mathbf{c}$	$(\mathbf{b}-\mathbf{a})$	$-(\mathbf{a}+\mathbf{b})$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmab$ $(\mathbf{b}'/4)$	L45
$(2\bar{1}\bar{1}0)$	$\mathbf{c}$	$-(\mathbf{a}+2\mathbf{b})$	$\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$	L24

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Auxiliary tables for Laue class $D_{6h}-6/mmm$

Centring type *P*

Orientation orbit $(hkil)$	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn\overline{m+n}0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m+n}mn0)$	$\mathbf{c}$	$m\mathbf{a}+(m+n)\mathbf{b}$	$-q\mathbf{a}+(p-q)\mathbf{b}$	$\mathbf{b}$	$-(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$
$(n\overline{m+n}m0)$	$\mathbf{c}$	$-(m+n)\mathbf{a}-n\mathbf{b}$	$(q-p)\mathbf{a}-p\mathbf{b}$	$-(\mathbf{a}+\mathbf{b})$	$\mathbf{a}$	$\mathbf{c}$
$(nm\overline{m+n}0)$	$-\mathbf{c}$	$m\mathbf{a}-n\mathbf{b}$	$-q\mathbf{a}-p\mathbf{b}$	$-\mathbf{b}$	$-\mathbf{a}$	$-\mathbf{c}$
$(\overline{m+n}nm0)$	$\mathbf{c}$	$n\mathbf{a}+(m+n)\mathbf{b}$	$p\mathbf{a}+(p-q)\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$-\mathbf{b}$	$-\mathbf{c}$
$(m\overline{m+n}n0)$	$-\mathbf{c}$	$-(m+n)\mathbf{a}-m\mathbf{b}$	$(q-p)\mathbf{a}+q\mathbf{b}$	$-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$-\mathbf{c}$
$(0h\bar{h}l)$	$\mathbf{a}$	$n(\mathbf{a}+2\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}+2\mathbf{b})+q\mathbf{c}$	$\mathbf{a}+2\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0h\bar{h}\bar{l})$	$-\mathbf{a}$	$n(\mathbf{a}+2\mathbf{b})+m\mathbf{c}$	$p(\mathbf{a}+2\mathbf{b})-q\mathbf{c}$			
$(\bar{h}0hl)$	$\mathbf{b}$	$-n(2\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$-p(2\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$-(2\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$\mathbf{b}$
$(\bar{h}0h\bar{l})$	$-\mathbf{b}$	$-n(2\mathbf{a}+\mathbf{b})+m\mathbf{c}$	$-p(2\mathbf{a}+\mathbf{b})-q\mathbf{c}$			
$(h\bar{h}0l)$	$-(\mathbf{a}+\mathbf{b})$	$n(\mathbf{a}-\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}-\mathbf{b})+q\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$
$(h\bar{h}0\bar{l})$	$(\mathbf{a}+\mathbf{b})$	$n(\mathbf{a}-\mathbf{b})+m\mathbf{c}$	$p(\mathbf{a}-\mathbf{b})-q\mathbf{c}$			
l odd $\Rightarrow n=l, m=2h$; l even $\Rightarrow n=l/2, m=h$						
$(\bar{h}2h\bar{h}l)$	$2\mathbf{a}+\mathbf{b}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$2\mathbf{a}+\mathbf{b}$
$(\bar{h}2h\bar{h}\bar{l})$	$-(2\mathbf{a}+\mathbf{b})$	$n\mathbf{b}+m\mathbf{c}$	$p\mathbf{b}-q\mathbf{c}$			
$(h\bar{h}2hl)$	$\mathbf{b}-\mathbf{a}$	$-n(\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$-p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$-(\mathbf{a}+\mathbf{b})$	$\mathbf{c}$	$\mathbf{b}-\mathbf{a}$
$(h\bar{h}2h\bar{l})$	$\mathbf{a}-\mathbf{b}$	$-n(\mathbf{a}+\mathbf{b})+m\mathbf{c}$	$-p(\mathbf{a}+\mathbf{b})-q\mathbf{c}$			
$(2h\bar{h}hl)$	$-(\mathbf{a}+2\mathbf{b})$	$n\mathbf{a}-m\mathbf{c}$	$p\mathbf{a}+q\mathbf{c}$	$\mathbf{a}$	$\mathbf{c}$	$-\mathbf{a}+2\mathbf{b}$
$(2h\bar{h}h\bar{l})$	$\mathbf{a}+2\mathbf{b}$	$n\mathbf{a}+m\mathbf{c}$	$p\mathbf{a}-q\mathbf{c}$			
l odd $\Rightarrow n=l, m=2h$; l even $\Rightarrow n=l/2, m=h$						

Arithmetic class 622*P*

Serial No.	177	178	179	180	181	182
Group type	D_6^1	D_6^2	D_6^3	D_6^4	D_6^5	D_6^6
Group	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$
$(mn\overline{m+n}0)$ $(\overline{m+n}mn0)$ $(n\overline{m+n}m0)$ $(nm\overline{m+n}0)$ $(\overline{m+n}nm0)$ $(m\overline{m+n}n0)$	$P112$	$P112_1$	$P112_1$	$P112$	$P112$	$P112_1$
	Reference group $B112$ with respect to origin at:					
$(0h\bar{h}l)$ $(0h\bar{h}\bar{l})$	P	P	P	P	P	P
$(\bar{h}0hl)$ $(\bar{h}0h\bar{l})$		$P+\mathbf{c}/3$	$P+\mathbf{c}/6$	$P+\mathbf{c}/6$	$P+\mathbf{c}/3$	
$(h\bar{h}0l)$ $(h\bar{h}0\bar{l})$		$P+\mathbf{c}/6$	$P+\mathbf{c}/3$	$P+\mathbf{c}/3$	$P+\mathbf{c}/6$	
$(\bar{h}2h\bar{h}l)$ $(\bar{h}2h\bar{h}\bar{l})$	P	$P+\mathbf{c}/12$	$P+5\mathbf{c}/12$	$P+\mathbf{c}/6$	$P+\mathbf{c}/3$	$P+\mathbf{c}/4$
$(\bar{h}h2hl)$ $(\bar{h}h2h\bar{l})$		$P+5\mathbf{c}/12$	$P+\mathbf{c}/12$	$P+\mathbf{c}/3$	$P+\mathbf{c}/6$	
$(2h\bar{h}hl)$ $(2h\bar{h}h\bar{l})$		$P+\mathbf{c}/4$	$P+\mathbf{c}/4$	P	P	

Arithmetic class $6mmP$

Serial No.	183	184	185	186
Group type	C_{6v}^1	C_{6v}^2	C_{6v}^3	C_{6v}^4
Group	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$
$(mn\overline{m+n}0)$ $(\overline{m+n}mn0)$ $(n\overline{m+n}m0)$ $(nm\overline{m+n}0)$ $(\overline{m+n}nm0)$ $(m\overline{m+n}n0)$	$P112$	$P112$	$P112_1$	$P112_1$
$(0h\overline{h}l)$ $(0h\overline{h}\overline{l})$ $(\overline{h}0hl)$ $(\overline{h}0h\overline{l})$ $(h\overline{h}0l)$ $(h\overline{h}0\overline{l})$	$B11m$	$B11b$	$B11b$	$B11m$
$(\overline{h}2h\overline{h}l)$ $(\overline{h}2h\overline{h}\overline{l})$ $(\overline{hh}2hl)$ $(\overline{hh}2h\overline{l})$ $(2h\overline{hh}l)$ $(2h\overline{hh}\overline{l})$	$B11m$	$B11b$	$B11m$	$B11b$

Arithmetic classes $\overline{6}m2P$ and $\overline{6}2mP$

Serial No.	187	188	189	190
Group type	D_{3h}^1	D_{3h}^2	D_{3h}^3	D_{3h}^4
Group	$P\overline{6}m2$	$P\overline{6}c2$	$P\overline{6}2m$	$P\overline{6}2c$
$(mn\overline{m+n}0)$ $(\overline{m+n}mn0)$ $(n\overline{m+n}m0)$ $(nm\overline{m+n}0)$ $(\overline{m+n}nm0)$ $(m\overline{m+n}n0)$	$P11m$	$P11m$ $(\mathbf{c}/4)$	$P11m$	$P11m$ $(\mathbf{c}/4)$
$(0h\overline{h}l)$ $(0h\overline{h}\overline{l})$ $(\overline{h}0hl)$ $(\overline{h}0h\overline{l})$ $(h\overline{h}0l)$ $(h\overline{h}0\overline{l})$	$B11m$	$B11b$	$B112$	$B112$
$(\overline{h}2h\overline{h}l)$ $(\overline{h}2h\overline{h}\overline{l})$ $(\overline{hh}2hl)$ $(\overline{hh}2h\overline{l})$ $(2h\overline{hh}l)$ $(2h\overline{hh}\overline{l})$	$B112$	$B112$	$B11m$	$B11b$

Arithmetic class $6/mmmP$

Serial No.	191	192	193	194
Group type	D^1_{6h}	D^2_{6h}	D^3_{6h}	D^4_{6h}
Group	$P6/mmm$	$P6/mcc$	$P6_3/mcm$	$P6_3/mmc$
$(mn\overline{m+n}0)$	$P112/m$	$P112/m$	$P112_1/m$	$P112_1/m$
$(\overline{m+n}mn0)$				
$(n\overline{m+n}m0)$				
$(nm\overline{m+n}0)$				
$(\overline{m+n}nm0)$				
$(m\overline{m+n}n0)$				
$(0h\overline{h}\overline{l})$	$B112/m$	$B112/b$	$B112/b$	$B112/m$
$(0h\overline{h}l)$				
$(\overline{h}0hl)$				
$(\overline{h}0h\overline{l})$				
$(h\overline{h}0l)$				
$(h\overline{h}0\overline{l})$				
$(\overline{h}2h\overline{h}\overline{l})$	$B112/m$	$B112/b$	$B112/m$	$B112/b$
$(\overline{h}2h\overline{h}l)$				
$(\overline{h\overline{h}}2hl)$				
$(\overline{h\overline{h}}2h\overline{l})$				
$(2h\overline{h\overline{h}}l)$				
$(2h\overline{h\overline{h}}\overline{l})$				

Note: vectors along cubic diagonals $[111]$, $[1\overline{1}\overline{1}]$, $[\overline{1}1\overline{1}]$ and $[\overline{1}\overline{1}1]$ are abbreviated as $\boldsymbol{\tau} = \mathbf{a}+\mathbf{b}+\mathbf{c}$, $\boldsymbol{\tau}_1 = \mathbf{a}-\mathbf{b}-\mathbf{c}$, $\boldsymbol{\tau}_2 = -\mathbf{a}+\mathbf{b}-\mathbf{c}$ and $\boldsymbol{\tau}_3 = -\mathbf{a}-\mathbf{b}+\mathbf{c}$, respectively, for cubic groups.

Laue class $T_h - m\overline{3}$

Geometric class T – 23

No. 195 $P23$ T^1

$$\mathcal{G} = P23$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P222$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p222$	L19
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112$	L03
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R3$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3$	L65
$(\overline{1}\overline{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$				
$(1\overline{1}\overline{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$				
$(\overline{1}1\overline{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$				

No. 196 $F23$ T^2

$$\mathcal{G} = F23$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222\ [(\mathbf{a}'+\mathbf{b}')/4]$	L22
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R3$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3$	L65
$(\overline{1}\overline{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$				
$(1\overline{1}\overline{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$				
$(\overline{1}1\overline{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$				

No. 197 $I23$ T^3

$$\mathcal{G} = I23$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\boldsymbol{\tau}/2$	$R3$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3$	L65
$(\overline{1}\overline{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_3/2$				
$(1\overline{1}\overline{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_1/2$				
$(\overline{1}1\overline{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\boldsymbol{\tau}_2/2$				

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No. 198 $P2_13$ T^4

$$\mathcal{G} = P2_13$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122\ (\mathbf{b}'/4)$	L20
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	τ	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	τ_3	With respect to origin at $P + (\mathbf{a} + \mathbf{c})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{b}$	$\mathbf{c} - \mathbf{b}$	τ_1	With respect to origin at $P + (\mathbf{b} + \mathbf{a})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	τ_2	With respect to origin at $P + (\mathbf{c} + \mathbf{b})/2$			
				$R3$	$[s\mathbf{d}, (s + \frac{1}{3})\mathbf{d}, (s + \frac{2}{3})\mathbf{d}]$	$p3$	L65

No. 199 $I2_13$ T^5

$$\mathcal{G} = I2_13$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2_122\ (\mathbf{b}'/4)$	L20
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{b}'/4)$	L20
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112\ (\mathbf{b}'/4)$	L03
(111)	$\mathbf{a} - \mathbf{c}$	$\mathbf{b} - \mathbf{a}$	$\tau/2$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$-\mathbf{a} - \mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\tau_3/2$	With respect to origin at $P + \mathbf{b}/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{c}$	$-\mathbf{a} - \mathbf{b}$	$\tau_1/2$	With respect to origin at $P + \mathbf{c}/2$			
$(\bar{1}1\bar{1})$	$\mathbf{c} - \mathbf{a}$	$\mathbf{a} + \mathbf{b}$	$\tau_2/2$	With respect to origin at $P + \mathbf{a}/2$			
				$R3$	$[s\mathbf{d}, (s + \frac{1}{3})\mathbf{d}, (s + \frac{2}{3})\mathbf{d}]$	$p3$	L65

Geometric class $T_h - m\bar{3}$

No. 200 $Pm\bar{3}$ T_h^1

$$\mathcal{G} = P\frac{2}{m}\bar{3}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Pmmm$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$pmmm$	L37
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[s\mathbf{d}, -s\mathbf{d}]$	$pmm2$	L23
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$				
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	τ	$R\bar{3}$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	τ_3		$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}' + \mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$	τ_1		$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}' + 2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	τ_2		$[\pm s\mathbf{d}, (\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 201 $Pn\bar{3}$ T_h^2

$$\mathcal{G} = P\tfrac{2}{n}\bar{3} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Pnnn$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 1)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p112/n\ [(\mathbf{a}'+\mathbf{b}')/4]$	L07
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R\bar{3}$	$[\frac{1}{4}\mathbf{d}, \quad [\frac{3}{4}\mathbf{d},$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	$(\mathbf{d}/4)$	$\frac{7}{12}\mathbf{d}, \parallel \frac{1}{12}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{11}{12}\mathbf{d}] \quad \frac{5}{12}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{4})\mathbf{d}, (\pm s+\frac{7}{12})\mathbf{d},$		
					$(\pm s+\frac{11}{12})\mathbf{d}]$	$p3$	L65

No. 201 $Pn\bar{3}$ T_h^2

$$\mathcal{G} = P\tfrac{2}{n}\bar{3} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Pnnn$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p112/n$	L07
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p222\ [(\mathbf{a}'+\mathbf{b}')/4]$	L19
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112\ [(\mathbf{a}'+\mathbf{b}')/4]$	L03
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/2$			
				$R\bar{3}$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
					$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

No. 202 $Fm\bar{3}$ T_h^3

$$\mathcal{G} = F\tfrac{2}{m}\bar{3}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Fmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cmmm$	L47
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cmme\ (\mathbf{b}'/4)$	L48
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$cmm2$	L26
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 203 $Fd\bar{3}$ T_h^4

$\mathcal{G} = F\frac{2}{d}\bar{3}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Fddd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$c222$	L22
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 1)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222\ [(\mathbf{a}'+\mathbf{b}')/4]$	L22
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{p}112/b\ [(\mathbf{a}'+\mathbf{b}')/8]$	L07
					$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{p}112/a\ [(3\mathbf{a}'+\mathbf{b}')/8$	
						or $(\mathbf{a}'+3\mathbf{b}')/8]$	L07
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$	L03
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}$	$[\frac{1}{8}\mathbf{d}, \quad [\frac{5}{8}\mathbf{d},$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	$(\mathbf{d}/8)$	$\frac{11}{24}\mathbf{d}, \parallel \frac{23}{24}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{19}{24}\mathbf{d}] \quad \frac{7}{24}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{8})\mathbf{d}, (\pm s+\frac{11}{24})\mathbf{d},$		
					$(\pm s+\frac{19}{24})\mathbf{d}]$	$p3$	L65

No. 203 $Fd\bar{3}$ T_h^4

$\mathcal{G} = F\frac{2}{d}\bar{3}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$Fddd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/b$	L07
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/a\ (\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L07
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222\ [(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222\ [3(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112\ [(\mathbf{a}'+\mathbf{b}')/8]$	L03
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/4$			
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/4$			
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/4$			
				$R\bar{3}$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
					$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 204 $Im\bar{3}$ T_h^5

$$\mathcal{G} = I\frac{2}{m}\bar{3}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	*Immm*	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	*pmmm*	L37
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	*pmmn* $[(\mathbf{a}'+\mathbf{b}')/4]$	L46
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	*pmm*2	L23
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\tau/2$	$R\bar{3}$	$[0\mathbf{d},\quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\tau_3/2$		$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\tau_1/2$		$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\tau_2/2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},\ (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

No. 205 $Pa\bar{3}$ T_h^6

$$\mathcal{G} = P\frac{2}{a}\bar{3}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	*Pbca*	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p2_1/b11$	L17
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pb2_1a$	L33
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pb11$ $(\mathbf{a}'/4)$	L12
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	τ	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	τ_3	With respect to origin at $P+(\mathbf{a}+\mathbf{c})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	τ_1	With respect to origin at $P+(\mathbf{b}+\mathbf{a})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	τ_2	With respect to origin at $P+(\mathbf{c}+\mathbf{b})/2$			
				$R\bar{3}$	$[0\mathbf{d},\quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
					$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},\ (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

No. 206 $Ia\bar{3}$ T_h^7

$$\mathcal{G} = I\frac{2}{a}\bar{3}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	*Ibca*	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	*pbab*	L43
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	*pbaa* $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	*pba*2 $(\mathbf{b}'/4)$	L25
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\tau/2$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\tau_3/2$	With respect to origin at $P+\mathbf{b}/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\tau_1/2$	With respect to origin at $P+\mathbf{c}/2$			
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\tau_2/2$	With respect to origin at $P+\mathbf{a}/2$			
				$R\bar{3}$	$[0\mathbf{d},\quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}$	L66
					$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},\ (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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Auxiliary tables for Laue class $T_h - m\bar{3}$

Centring types *P* and *I*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\overline{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(n0\overline{m})$	$\mathbf{b}$	$n\mathbf{c}+m\mathbf{a}$	$-p\mathbf{c}+q\mathbf{a}$			

Arithmetic classes $23P$ and $23I$

Serial No.	195	198	197	199
Group type	T^1	T^4	T^3	T^5
Group	$P23$	$P2_13$	$I23$	$I2_13$
$(mn0)$	$P112$	$P112_1$	$I112$	$I112$
$(\overline{m}n0)$		$(\mathbf{a}/4)$		$(\mathbf{b}/4)$
$(0mn)$		$P112_1$		$I112$
$(0\overline{m}n)$		$(\mathbf{b}/4)$		$(\mathbf{c}/4)$
$(n0m)$		$P112_1$		$I112$
$(n0\overline{m})$		$(\mathbf{c}/4)$		$(\mathbf{a}/4)$

Arithmetic classes $m\bar{3}P$ and $m\bar{3}I$

Serial No.	200	201		205	204	206
Group type	T_h^1	T_h^2		T_h^6	T_h^5	T_h^7
Group	$Pm\bar{3}$	$Pn\bar{3}$		$Pa\bar{3}$	$Im\bar{3}$	$Ia\bar{3}$
		Origin 1	Origin 2			
$(mn0)$	$P112/m$	$P112/n$	$P112/n$	$P112_1/a$	$I112/m$	$I112/b$
$(\overline{m}n0)$		$(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$				
$(0mn)$						
$(0\overline{m}n)$						
$(n0m)$						
$(n0\overline{m})$						

Centring type *F*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(hk0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$
$(\bar{h}k0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
$(0hk)$	$\mathbf{a}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$
$(0\bar{h}k)$	$\mathbf{a}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
$(k0h)$	$\mathbf{b}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$
$(k0\bar{h})$	$\mathbf{b}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
h even, k odd or h odd, k even $\Rightarrow n = h + k, m = h - k$ h, k odd $\Rightarrow n = (h + k)/2, m = (h - k)/2$						

Arithmetic classes $23F$ and $m\bar{3}F$

Serial No.	196	202	203	
Group type	T^2	T_h^3	T_h^4	
Group	$F23$	$Fm\bar{3}$	$Fd\bar{3}$	
			Origin 1	Origin 2
$(hk0)$ $(\bar{h}k0)$ $(0hk)$ $(0\bar{h}k)$ $(k0h)$ $(k0\bar{h})$	$I112$	$I112/m$	$I112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/b$

Laue class $O_h - m\bar{3}m$

Geometric class O – 432

No. 207 $P432$ O^1

$$\mathcal{G} = P432$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P422$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p422$	L53
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p4$	L49
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$				
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$A222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$	L20
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R32$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p321$	L68
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p321\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}1)$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p321\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 208 $P4_232$ O^2

$$\mathcal{G} = P4_232$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_222$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p222$	L19
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$(\mathbf{a}'/2$ or $\mathbf{b}'/2)$	$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$ $(\mathbf{a}'/2$ or $\mathbf{b}'/2)$	L22
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$A222$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p22_12$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L20
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L19
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L03
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R32$	$[\frac{1}{4}\mathbf{d},\quad [\frac{3}{4}\mathbf{d},$	$p321$	L68
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	$(\mathbf{d}/4)$	$\frac{7}{12}\mathbf{d},\ \|\ \frac{1}{12}\mathbf{d},$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{11}{12}\mathbf{d}]\quad \frac{5}{12}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{4})\mathbf{d},\ (\pm s+\frac{7}{12})\mathbf{d},$		
					$(\pm s+\frac{11}{12})\mathbf{d}]$	$p3$	L65

No. 209 $F432$ O^3

$$\mathcal{G} = F432$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I422$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p422$	L53
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p42_12$	L54
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$I222$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p222$	L19
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p2_12_12$	L21
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$	L03
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$				
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$				
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R32$	$[0\mathbf{d},\quad [\frac{1}{2}\mathbf{d},$	$p321$	L68
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d},\ \|\ \frac{5}{6}\mathbf{d},$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}]\quad \frac{1}{6}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 210 $F4_132$ O^4

$$\mathcal{G} = F4_132$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{c}222$	L22
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$		$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}222$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L22
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p22_12$	L20
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_122$	L20
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$p112$	L03
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L20
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	($3\mathbf{a}'/8+\mathbf{d}/4$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L20
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L03
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$	$I2_12_12_1$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p22_12$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L20
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$	($\mathbf{a}'/8+\mathbf{d}/4$)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_122$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L20
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p112$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L03
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R32$	$[\frac{1}{8}\mathbf{d},$ $[\frac{5}{8}\mathbf{d},$	$p321$	L68
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	($\mathbf{d}/8$)	$\frac{11}{24}\mathbf{d},$ $\parallel$ $\frac{23}{24}\mathbf{d},$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{19}{24}\mathbf{d}]$ $\frac{7}{24}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{8})\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{19}{24})\mathbf{d}]$	$p3$	L65

No. 211 $I432$ O^5

$$\mathcal{G} = I432$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I422$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p422$	L53
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p42_12$	L54
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$F222$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c222$	L22
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c222$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L22
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{p}112$	L03
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\boldsymbol{\tau}/2$	$R32$	$[0\mathbf{d},$ $[\frac{1}{2}\mathbf{d},$	$p321$	L68
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_3/2$		$\frac{1}{3}\mathbf{d},$ $\parallel$ $\frac{5}{6}\mathbf{d},$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_1/2$		$\frac{2}{3}\mathbf{d}]$ $\frac{1}{6}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\boldsymbol{\tau}_2/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3$	L65

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No. 212 $P4_332$ O^6

$$\mathcal{G} = P4_332$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_32_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p2_111$ $(\mathbf{b}'/4)$	L09
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$(\mathbf{a}'/4 + 3\mathbf{d}/8)$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_111$	L09
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{c}211$ $(\mathbf{a}'/4)$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{c}121$ $(\mathbf{a}'/4)$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(110)	$\mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$A2_122$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$p2_122$ $[(3\mathbf{a}' + \mathbf{b}')/8]$	L20
(011)	$\mathbf{a}$	$\mathbf{b} - \mathbf{c}$	$\mathbf{b} + \mathbf{c}$	$[(\mathbf{a}' + \mathbf{b}' + \mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_12_12$ $[(3\mathbf{a}' + \mathbf{b}')/8]$	L21
(101)	$\mathbf{b}$	$\mathbf{c} - \mathbf{a}$	$\mathbf{c} + \mathbf{a}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$p112$ $[(3\mathbf{a}' + \mathbf{b}')/8]$	L03
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a} + \mathbf{b}$	$\mathbf{b} - \mathbf{a}$	$A2_122$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$p2_12_12$ $[(\mathbf{a}' + \mathbf{b}')/8]$	L21
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$	$[(\mathbf{a}' + \mathbf{b}' + 3\mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_122$ $[(\mathbf{a}' + \mathbf{b}')/8]$	L20
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c} + \mathbf{a}$	$\mathbf{a} - \mathbf{c}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$p112$ $[(\mathbf{a}' + \mathbf{b}')/8]$	L03
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P + (\mathbf{a} + \mathbf{c})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{b}$	$\mathbf{c} - \mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P + (\mathbf{b} + \mathbf{a})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P + (\mathbf{c} + \mathbf{b})/2$			
				$R32$	$[\frac{1}{8}\mathbf{d}, \quad [\frac{5}{8}\mathbf{d},$	$p321$	L68
				$(\mathbf{d}/8)$	$\frac{11}{24}\mathbf{d}, \ \| \ \frac{23}{24}\mathbf{d},$	$p321$ $[(2\mathbf{a}' + \mathbf{b}')/3]$	L68
					$\frac{19}{24}\mathbf{d}] \quad \frac{7}{24}\mathbf{d}]$	$p321$ $[(\mathbf{a}' + 2\mathbf{b}')/3]$	L68
					$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{11}{24})\mathbf{d},$		
					$(\pm s + \frac{19}{24})\mathbf{d}]$	$p3$	L65

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No. 213 $P4_132$ O^7

$$\mathcal{G} = P4_132$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_12_12$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p2_111$ $(\mathbf{b}'/4)$	L09
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$(3\mathbf{a}'/4 + \mathbf{d}/8)$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p12_11$	L09
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{c}121$ $(3\mathbf{a}'/4)$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{c}211$ $(3\mathbf{a}'/4)$	L10
					$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{3}{8})\mathbf{d},$		
					$(\pm s + \frac{5}{8})\mathbf{d}, (\pm s + \frac{7}{8})\mathbf{d}]$	$p1$	L01
(110)	$\mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$A2_122$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$p2_12_12$ $[(\mathbf{a}'+3\mathbf{b}')/8]$	L21
(011)	$\mathbf{a}$	$\mathbf{b} - \mathbf{c}$	$\mathbf{b} + \mathbf{c}$	$[3(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_122$ $[(\mathbf{a}' + 3\mathbf{b}')/8]$	L20
(101)	$\mathbf{b}$	$\mathbf{c} - \mathbf{a}$	$\mathbf{c} + \mathbf{a}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$p112$ $[(\mathbf{a}' + 3\mathbf{b}')/8]$	L03
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a} + \mathbf{b}$	$\mathbf{b} - \mathbf{a}$	$A2_122$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$p2_122$ $[3(\mathbf{a}' + \mathbf{b}')/8]$	L20
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$	$[(\mathbf{a}'+3\mathbf{b}'+\mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p2_12_12$ $[3(\mathbf{a}'+\mathbf{b}')/8]$	L21
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c} + \mathbf{a}$	$\mathbf{a} - \mathbf{c}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$p112$ $[3(\mathbf{a}' + \mathbf{b}')/8]$	L03
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P + (\mathbf{a} + \mathbf{c})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{b}$	$\mathbf{c} - \mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P + (\mathbf{b} + \mathbf{a})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P + (\mathbf{c} + \mathbf{b})/2$			
				$R32$	$[\frac{3}{8}\mathbf{d}, \quad [\frac{7}{8}\mathbf{d},$	$p321$	L68
				$(3\mathbf{d}/8)$	$\frac{17}{24}\mathbf{d}, \parallel \frac{5}{24}\mathbf{d},$	$p321$ $[(2\mathbf{a}' + \mathbf{b}')/3]$	L68
					$\frac{1}{24}\mathbf{d}] \quad \frac{13}{24}\mathbf{d}]$	$p321$ $[(\mathbf{a}' + 2\mathbf{b}')/3]$	L68
					$[(\pm s + \frac{3}{8})\mathbf{d}, (\pm s + \frac{17}{24})\mathbf{d},$		
					$(\pm s + \frac{1}{24})\mathbf{d}]$	$p3$	L65

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No. 214 $I4_132$ O^8

$$\mathcal{G} = I4_132$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I4_122$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p2_122\ (\mathbf{b}'/4)$	L20
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$(\mathbf{b}'/4 + \mathbf{d}/8)$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12\ (\mathbf{b}'/4)$	L20
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$\widehat{c}222\ (\mathbf{b}'/4)$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$\widehat{c}222\ (3\mathbf{b}'/4)$	L22
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p112\ (\mathbf{b}'/4)$	L03
(110)	$\mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$F222$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$c222\ [(\mathbf{a}' + 3\mathbf{b}')/8]$	L22
(011)	$\mathbf{a}$	$\mathbf{b} - \mathbf{c}$	$\mathbf{b} + \mathbf{c}$	$[(\mathbf{a}'+3\mathbf{b}'+\mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222\ [(3\mathbf{a}' + \mathbf{b}')/8]$	L22
(101)	$\mathbf{b}$	$\mathbf{c} - \mathbf{a}$	$\mathbf{c} + \mathbf{a}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$\widehat{p}112\ [(\mathbf{a}' + 3\mathbf{b}')/8]$	L03
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a} + \mathbf{b}$	$\mathbf{b} - \mathbf{a}$	$F222$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d}]$	$c222\ [(\mathbf{a}' + \mathbf{b}')/8]$	L22
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$	$[(\mathbf{a}' + \mathbf{b}' + \mathbf{d})/8]$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222\ [3(\mathbf{a}' + \mathbf{b}')/8]$	L22
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c} + \mathbf{a}$	$\mathbf{a} - \mathbf{c}$		$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{5}{8})\mathbf{d}]$	$\widehat{p}112\ [(\mathbf{a}' + \mathbf{b}')/8]$	L03
(111)	$\mathbf{a} - \mathbf{c}$	$\mathbf{b} - \mathbf{a}$	$\boldsymbol{\tau}/2$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$-\mathbf{a} - \mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\boldsymbol{\tau}_3/2$	With respect to origin at $P + \mathbf{b}/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{c}$	$-\mathbf{a} - \mathbf{b}$	$\boldsymbol{\tau}_1/2$	With respect to origin at $P + \mathbf{c}/2$			
$(\bar{1}1\bar{1})$	$\mathbf{c} - \mathbf{a}$	$\mathbf{a} + \mathbf{b}$	$\boldsymbol{\tau}_2/2$	With respect to origin at $P + \mathbf{a}/2$			
				$R32$	$[\frac{1}{8}\mathbf{d}, \quad [\frac{5}{8}\mathbf{d},$	$p321$	L68
				$(\mathbf{d}/8)$	$\frac{11}{24}\mathbf{d}, \ \| \ \frac{23}{24}\mathbf{d},$	$p321\ [(2\mathbf{a}' + \mathbf{b}')/3]$	L68
					$\frac{19}{24}\mathbf{d}] \quad \frac{7}{24}\mathbf{d}]$	$p321\ [(\mathbf{a}' + 2\mathbf{b}')/3]$	L68
					$[(\pm s + \frac{1}{8})\mathbf{d}, (\pm s + \frac{11}{24})\mathbf{d},$		
					$(\pm s + \frac{19}{24})\mathbf{d}]$	$p3$	L65

Geometric class $T_d - \bar{4}3m$

No. 215 $P\bar{4}3m$ T_d^1

$$\mathcal{G} = P\bar{4}3m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}2m$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p\bar{4}2m$	L57
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[s\mathbf{d}, -s\mathbf{d}]$	$\widehat{c}mm2$	L26
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$				
(110)	$\mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$A2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a} + \mathbf{b}$	$\mathbf{b} - \mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2mb\ (\mathbf{b}'/4)$	L31
(011)	$\mathbf{a}$	$\mathbf{b} - \mathbf{c}$	$\mathbf{b} + \mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c} - \mathbf{a}$	$\mathbf{c} + \mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c} + \mathbf{a}$	$\mathbf{a} - \mathbf{c}$				
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}$	$R3m$	$[s\mathbf{d}, (s + \frac{1}{3})\mathbf{d}, (s + \frac{2}{3})\mathbf{d}]$	$p3m1$	L69
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}_3$				
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{b}$	$\mathbf{c} - \mathbf{b}$	$\boldsymbol{\tau}_1$				
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	$\boldsymbol{\tau}_2$				

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No. 216 $F\bar{4}3m$ T_d^2

$$\mathcal{G} = F\bar{4}3m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I\bar{4}m2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}m2$	L59
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L59
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$I2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2mm$	L27
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1mn$	L32
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p1m1$	L11
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$				
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$				
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R3m$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$				
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$				
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$				

No. 217 $I\bar{4}3m$ T_d^3

$$\mathcal{G} = I\bar{4}3m$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I\bar{4}2m$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}2m$	L57
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2_1m$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L58
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$F2mm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$c2mm$	L35
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$c2me$ ($\mathbf{b}'/4$)	L36
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$c1m1$	L13
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\boldsymbol{\tau}/2$	$R3m$	$[s\mathbf{d}, (s+\frac{1}{3})\mathbf{d}, (s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_3/2$				
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_1/2$				
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\boldsymbol{\tau}_2/2$				

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No. 218 $P\bar{4}3n$ T_d^4

$$\mathcal{G} = P\bar{4}3n$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{4}2c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p222$	L19
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$[(\mathbf{a}'/2 + \mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L50
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	or $(\mathbf{b}'/2 + \mathbf{d}/4)]$	$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p112$	L03
(110)	$\mathbf{c}$	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$A2aa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2an$	L34
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a} + \mathbf{b}$	$\mathbf{b} - \mathbf{a}$	$[(\mathbf{b}' + \mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2aa$ ($\mathbf{b}'/4$)	L30
(011)	$\mathbf{a}$	$\mathbf{b} - \mathbf{c}$	$\mathbf{b} + \mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1a1$ ($\mathbf{b}'/4$)	L05
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b} + \mathbf{c}$	$\mathbf{c} - \mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c} - \mathbf{a}$	$\mathbf{c} + \mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c} + \mathbf{a}$	$\mathbf{a} - \mathbf{c}$				
(111)	$\mathbf{a} - \mathbf{b}$	$\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}$	$R3c$	$[s\mathbf{d}, (s + \frac{1}{6})\mathbf{d},$		
$(\bar{1}\bar{1}1)$	$\mathbf{b} - \mathbf{a}$	$-\mathbf{b} - \mathbf{c}$	$\boldsymbol{\tau}_3$		$(s + \frac{1}{3})\mathbf{d}, (s + \frac{1}{2})\mathbf{d},$		
$(1\bar{1}\bar{1})$	$\mathbf{a} + \mathbf{b}$	$\mathbf{c} - \mathbf{b}$	$\boldsymbol{\tau}_1$		$(s + \frac{2}{3})\mathbf{d}, (s + \frac{5}{6})\mathbf{d}]$	$p3$	L65
$(\bar{1}1\bar{1})$	$-\mathbf{a} - \mathbf{b}$	$\mathbf{b} + \mathbf{c}$	$\boldsymbol{\tau}_2$				

No. 219 $F\bar{4}3c$ T_d^5

$$\mathcal{G} = F\bar{4}3c$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a} - \mathbf{b})/2$	$(\mathbf{a} + \mathbf{b})/2$	$\mathbf{c}$	$I\bar{4}c2$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}b2$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L60
(100)	$(\mathbf{b} - \mathbf{c})/2$	$(\mathbf{b} + \mathbf{c})/2$	$\mathbf{a}$	$(\mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$	L60
(010)	$(\mathbf{c} - \mathbf{a})/2$	$(\mathbf{c} + \mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pba2$	L25
(110)	$\mathbf{c}$	$(\mathbf{a} - \mathbf{b})/2$	$(\mathbf{a} + \mathbf{b})/2$	$I2cb$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p2aa$	L30
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a} + \mathbf{b})/2$	$(\mathbf{b} - \mathbf{a})/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p2_1ab$ ($\mathbf{b}'/4$)	L33
(011)	$\mathbf{a}$	$(\mathbf{b} - \mathbf{c})/2$	$(\mathbf{b} + \mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1a1$	L12
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b} + \mathbf{c})/2$	$(\mathbf{c} - \mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c} - \mathbf{a})/2$	$(\mathbf{c} + \mathbf{a})/2$				
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c} + \mathbf{a})/2$	$(\mathbf{a} - \mathbf{c})/2$				
(111)	$(\mathbf{a} - \mathbf{c})/2$	$(\mathbf{b} - \mathbf{a})/2$	$\boldsymbol{\tau}$	$R3c$	$[s\mathbf{d}, (s + \frac{1}{6})\mathbf{d},$		
$(\bar{1}\bar{1}1)$	$(-\mathbf{a} - \mathbf{c})/2$	$(\mathbf{a} - \mathbf{b})/2$	$\boldsymbol{\tau}_3$		$(s + \frac{1}{3})\mathbf{d}, (s + \frac{1}{2})\mathbf{d},$		
$(1\bar{1}\bar{1})$	$(\mathbf{a} + \mathbf{c})/2$	$(-\mathbf{a} - \mathbf{b})/2$	$\boldsymbol{\tau}_1$		$(s + \frac{2}{3})\mathbf{d}, (s + \frac{5}{6})\mathbf{d}]$	$p3$	L65
$(\bar{1}1\bar{1})$	$(\mathbf{c} - \mathbf{a})/2$	$(\mathbf{a} + \mathbf{b})/2$	$\boldsymbol{\tau}_2$				

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No. 220 $I\bar{4}3d$ T_d^6

$\mathcal{G} = I\bar{4}3d$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I\bar{4}2d$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p2_122$ $(\mathbf{b}'/4)$	L20
(100)	**b**	**c**	**a**	$(3\mathbf{b}'/4 + \mathbf{d}/8)$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p22_12$ $(\mathbf{b}'/4)$	L20
(010)	**c**	**a**	**b**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}$ $(3\mathbf{b}'/4)$	L50
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}$ $(\mathbf{b}'/4)$	L50
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p112$	L03
(110)	**c**	**a** − **b**	**a** + **b**	$F2dd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}11a$	L05
(011)	**a**	**b** − **c**	**b** + **c**	$[(3\mathbf{b}' + \mathbf{d})/8]$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}11b$	L05
(101)	**b**	**c** − **a**	**c** + **a**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c211$ $(3\mathbf{b}'/8)$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c211$ $(\mathbf{b}'/8)$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
$(1\bar{1}0)$	**c**	**a** + **b**	**b** − **a**	$F2dd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}11b$	L05
$(01\bar{1})$	**a**	**b** + **c**	**c** − **b**	$[3(\mathbf{b}' + \mathbf{d})/8]$	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}11a$	L05
$(\bar{1}01)$	**b**	**c** + **a**	**a** − **c**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c211$ $(\mathbf{b}'/8)$	L10
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c211$ $(3\mathbf{b}'/8)$	L10
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d},$		
					$(\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$	$p1$	L01
(111)	**a** − **c**	**b** − **a**	$\boldsymbol{\tau}/2$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	−**a** − **c**	**a** − **b**	$\boldsymbol{\tau}_3/2$	With respect to origin at $P + (\mathbf{a} + \mathbf{c})/2$			
$(1\bar{1}\bar{1})$	**a** + **c**	−**a** − **b**	$\boldsymbol{\tau}_1/2$	With respect to origin at $P + (\mathbf{b} + \mathbf{a})/2$			
$(\bar{1}1\bar{1})$	**c** − **a**	**a** + **b**	$\boldsymbol{\tau}_2/2$	With respect to origin at $P + (\mathbf{c} + \mathbf{b})/2$			
				$R3c$	$[s\mathbf{d}, (s + \frac{1}{6})\mathbf{d},$		
					$(s + \frac{1}{3})\mathbf{d}, (s + \frac{1}{2})\mathbf{d},$		
					$(s + \frac{2}{3})\mathbf{d}, (s + \frac{5}{6})\mathbf{d}]$	$p3$	L65

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Geometric class $O_h - m\bar{3}m$

No. 221 $Pm\bar{3}m$ O_h^1

$$\mathcal{G} = P\frac{4}{m}\bar{3}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/mmm$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p4/mmm$	L61
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p4mm$	L55
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$				
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Ammm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmb$ $(\mathbf{b}'/4)$	L41
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R\bar{3}m$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69

No. 222 $Pn\bar{3}n$ O_h^2

$$\mathcal{G} = P\frac{4}{n}\bar{3}\frac{2}{n} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/nnc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p422$	L53
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 1)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/n$	L52
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4$	L49
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Abaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L39
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	(origin 1)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $(\mathbf{a}'/4)$	L43
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$	L25
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R\bar{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p321$	L68
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	$(\mathbf{d}/4)$	$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$p\bar{3}$	L66
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p3$	L65

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No. 222 $Pn\overline{3}n$ O_h^2

$\mathcal{G} = P\frac{4}{n}\overline{3}\frac{2}{n}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4/nnc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/n\ [(\mathbf{a}'+\mathbf{b}')/4]$	L52
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p422\ [(\mathbf{a}'+\mathbf{b}')/4]$	L53
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4\ [(\mathbf{a}'+\mathbf{b}')/4]$	L49
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Abaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbaa$	L43
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$	(origin 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pban\ (\mathbf{b}'/4)$	L39
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2\ (\mathbf{a}'/4)$	L25
$(1\overline{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$Abaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pban$	L39
$(01\overline{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$	(origin 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa\ (\mathbf{b}'/4)$	L43
$(\overline{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$	$[(\mathbf{b}'+\mathbf{d})/4]$	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2\ [(\mathbf{a}'+\mathbf{b}')/4]$	L25
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\overline{1}\overline{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/2$			
$(1\overline{1}\overline{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/2$			
$(\overline{1}1\overline{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/2$			
				$R\overline{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\overline{3}$	L66
					$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$p\overline{3}\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$p\overline{3}\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$p321$	L68
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$p321\ [(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$p321\ [(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p3$	L65

No. 223 $Pm\bar{3}n$ O_h^3

$$\mathcal{G} = P\frac{4_2}{m}\bar{3}\frac{2}{n}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/mmc$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	$(\mathbf{a}'/2$ or $\mathbf{b}'/2)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$ $(\mathbf{a}'/2$ or $\mathbf{b}'/2)$	L59
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pmm2$	L23
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Amaa$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pman$	L42
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$[(\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmaa$ $(\mathbf{b}'/4)$	L38
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pma2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R\bar{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$p321$	L68
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{6})\mathbf{d},$		
					$(\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d},$		
					$(\pm s + \frac{2}{3})\mathbf{d}, (\pm s + \frac{5}{6})\mathbf{d}]$	$p3$	L65

No. 224 $Pn\bar{3}m$ O_h^4

$$\mathcal{G} = P\frac{4_2}{n}\bar{3}\frac{2}{m} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/nnm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{4}2m$	L57
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 1)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{c}mme$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L48
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$	L26
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Abmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmm$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L40
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmb$ $(\mathbf{a}'/4)$	L38
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$pbm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	$R\bar{3}m$	$[\frac{1}{4}\mathbf{d},$ $[\frac{3}{4}\mathbf{d},$	$p\bar{3}m1$	L72
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	$(\mathbf{d}/4)$	$\frac{7}{12}\mathbf{d},$ $\|$ $\frac{1}{12}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$		$\frac{11}{12}\mathbf{d}]$ $\frac{5}{12}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{4})\mathbf{d}, (\pm s+\frac{7}{12})\mathbf{d}, (\pm s+\frac{11}{12})\mathbf{d}]$	$p3m1$	L69

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No. 224 $Pn\bar{3}m$ O_h^4

$$\mathcal{G} = P\frac{4_2}{n}\bar{3}\frac{2}{m} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/nnm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$\widehat{c}mme$	L48
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 2)	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}2m$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L57
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$(\mathbf{a}'/2$ or $\mathbf{b}'/2)$	$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$\widehat{c}mm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L26
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Abmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmb$	L38
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmm$ $(\mathbf{b}'/4)$	L40
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $(\mathbf{b}'/4)$	L24
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$Abmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmm$	L40
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$	$[(\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmb$ $(\mathbf{b}'/4)$	L38
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$	L24
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/2$			
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/2$			
$(\bar{1}1\bar{1})$	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/2$			
				$R\bar{3}m$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
					$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
					$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69

No. 225 $Fm\bar{3}m$ O_h^5

$$\mathcal{G} = F\frac{4}{n}\bar{3}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4/mmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/mmm$	L61
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/nmm$	L64
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$p4mm$	L55
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Immm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pmmm$	L37
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmmn$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L46
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pmm2$	L23
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$				
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$				
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}m$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69

No. 226 $Fm\bar{3}c$ O_h^6

$$\mathcal{G} = F\,\frac{4}{n}\,\bar{3}\,\frac{2}{c}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4/mcm$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$p4/mbm$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L633
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p4/nbm$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L62
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$p4bm$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L56
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Imcb$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$pmaa$	L38
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pmab$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L45
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pma2$ ($\mathbf{a}'/4$)	L24
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$				
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$				
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}c$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d};$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$		$\frac{1}{3}\mathbf{d},\ \frac{5}{6}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{2}{3}\mathbf{d},\ \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d};$	$p321$	L68
					$\frac{1}{12}\mathbf{d},\ \frac{7}{12}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{5}{12}\mathbf{d},\ \frac{11}{12}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d},\ (\pm s+\frac{5}{6})\mathbf{d}]$	$p3$	L65

No. 227 $Fd\bar{3}m$ O_h^7

$$\mathcal{G} = F\,\frac{4_1}{d}\,\bar{3}\,\frac{2}{m} \quad \text{origin 1}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4_1/amd$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d};$	$p\bar{4}m2$	L59
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	(origin 1)	$\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$p\bar{4}m2$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L59
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d},\ \frac{5}{8}\mathbf{d};$	$pmmb$ ($\mathbf{b}'/4$)	L41
					$\frac{3}{8}\mathbf{d},\ \frac{7}{8}\mathbf{d}]$	$pmma$ ($\mathbf{a}'/4$)	L41
					$[\pm s\mathbf{d},\ (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d},\ (\pm s+\frac{3}{4})\mathbf{d}]$	$pmm2$	L23
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Ibmm$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$pbmm$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L40
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	($\mathbf{a}'/8+\mathbf{d}/4$)	$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pbmn$ ($\mathbf{a}'/8$)	L42
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L24
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$	$Ibmm$	$[0\mathbf{d},\ \frac{1}{2}\mathbf{d}]$	$pbmm$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L40
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$	($3\mathbf{a}'/8+\mathbf{d}/4$)	$[\frac{1}{4}\mathbf{d},\ \frac{3}{4}\mathbf{d}]$	$pbmn$ ($3\mathbf{a}'/8$)	L42
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$		$[\pm s\mathbf{d},\ (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L24
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}m$	$[\frac{1}{8}\mathbf{d},\quad [\frac{5}{8}\mathbf{d},$	$p\bar{3}m1$	L72
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	($\mathbf{d}/8$)	$\frac{11}{24}\mathbf{d},\ \|\ \frac{23}{24}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{19}{24}\mathbf{d}]\quad \frac{7}{24}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[(\pm s+\frac{1}{8})\mathbf{d},\ (\pm s+\frac{11}{24})\mathbf{d},$		
					$(\pm s+\frac{19}{24})\mathbf{d}]$	$p3m1$	L69

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No. 227 $Fd\bar{3}m$ O_h^7

$\mathcal{G} = F\frac{4_1}{d}\bar{3}\frac{2}{m}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4_1/amd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$pmmb$	L41
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pmma$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L41
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$	($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}m2$ $(\mathbf{b}'/4)$	L59
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}m2$ $(\mathbf{b}'/4)$	L59
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pmm2$ $(\mathbf{b}'/4)$	L23
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Ibmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmn$	L42
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmm$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L40
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L24
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$	$Ibmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbmm$	L40
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$	$[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbmn$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L42
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$	L24
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/4$			
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/4$			
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/4$			
				$R\bar{3}m$	$[0\mathbf{d}, \quad [\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
					$\frac{1}{3}\mathbf{d}, \parallel \frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
					$\frac{2}{3}\mathbf{d}] \quad \frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69

International Tables for Crystallography (2010). Vol. E, Scanning table for space group 228, pp. 553–554.

No. 228 $Fd\bar{3}c$ O_h^8

$\mathcal{G} = F\frac{4_1}{d}\bar{3}\frac{2}{c}$ origin 1

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4_1/acd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{4}b2$ ($\mathbf{a}'/2$ or $\mathbf{b}'/2$)	L60
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	(origin 1)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p\bar{4}b2$	L60
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$	$(\mathbf{d}/4)$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$pbaa$ ($\mathbf{a}'/4$)	L43
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$pbab$ ($\mathbf{b}'/4$)	L43
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pba2$	L25
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Ibca$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbaa$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L43
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$(3\mathbf{a}'/8+\mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ ($3\mathbf{a}'/8$)	L43
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L25
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$	$Ibca$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbaa$ ($3\mathbf{a}'/8+\mathbf{b}'/4$)	L43
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$	$(\mathbf{a}'/8+\mathbf{d}/4)$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ ($\mathbf{a}'/8$)	L43
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pbm2$ ($\mathbf{a}'/8+\mathbf{b}'/4$)	L24
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\bar{3}c$	$[\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d};$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	$(3\mathbf{d}/8)$	$\frac{17}{24}\mathbf{d}, \frac{5}{24}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\frac{1}{24}\mathbf{d}, \frac{13}{24}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\frac{5}{8}\mathbf{d}, \frac{1}{8}\mathbf{d};$	$p321$	L68
					$\frac{11}{24}\mathbf{d}, \frac{23}{24}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{19}{24}\mathbf{d}, \frac{7}{24}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[(\pm s+\frac{3}{8})\mathbf{d}, (\pm s+\frac{13}{24})\mathbf{d},$		
					$(\pm s+\frac{17}{24})\mathbf{d}, (\pm s+\frac{7}{8})\mathbf{d},$		
					$(\pm s+\frac{1}{24})\mathbf{d}, (\pm s+\frac{5}{24})\mathbf{d}]$	$p3$	L65

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No. 228 $Fd\bar{3}c$ O_h^8

$\mathcal{G} = F\frac{4_1}{d}\bar{3}\frac{2}{c}$ origin 2

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4_1/acd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$pbab$	L43
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}b2$ $(\mathbf{b}'/4)$	L60
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}b2$ $(\mathbf{b}'/4)$	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Ibca$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbab$	L43
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
$(1\bar{1}0)$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$	$Ibca$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$pbaa$	L43
$(01\bar{1})$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$	$[(\mathbf{a}'+\mathbf{b}'+\mathbf{d})/4]$	$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbab$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
$(\bar{1}01)$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d}]$	$pba2$ $(\mathbf{a}'/4)$	L25
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	With respect to origin at P			
$(\bar{1}\bar{1}1)$	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/4$			
$(1\bar{1}\bar{1})$	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/4$			
$(\bar{1}1\bar{1})$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/4$			
				$R\bar{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{3}$	L66
					$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
					$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$p321$	L68
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p3$	L65

No. 229 $Im\bar{3}m$ O_h^9

$$\mathcal{G} = I\frac{4}{m}\bar{3}\frac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$I4/mmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p4/mmm$	L61
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p4/nmm$	L64
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p4mm$	L55
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Fmmm$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$cmmm$	L47
$(1\bar{1}0)$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$cmme$ $(\mathbf{b}'/4)$	L48
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$cmm2$	L26
$(01\bar{1})$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$				
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$				
$(\bar{1}01)$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$				
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\boldsymbol{\tau}/2$	$R\bar{3}m$	$[0\mathbf{d},$ $[\frac{1}{2}\mathbf{d},$	$p\bar{3}m1$	L72
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_3/2$		$\frac{1}{3}\mathbf{d},$ $\parallel$ $\frac{5}{6}\mathbf{d},$	$p\bar{3}m1$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\boldsymbol{\tau}_1/2$		$\frac{2}{3}\mathbf{d}]$ $\frac{1}{6}\mathbf{d}]$	$p\bar{3}m1$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\boldsymbol{\tau}_2/2$		$[\pm s\mathbf{d}, (\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{2}{3})\mathbf{d}]$	$p3m1$	L69

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International Tables for Crystallography (2010). Vol. E, Scanning table for space group 230, p. 556.

No. 230 $Ia\bar{3}d$ O_h^{10}

$$\mathcal{G} = I\frac{4_1}{a}\bar{3}\frac{2}{d}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	**a**	**b**	**c**	$I4_1/acd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$pbab$	L43
(100)	**b**	**c**	**a**	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$pbaa$ $[(\mathbf{a}'+\mathbf{b}')/4]$	L43
(010)	**c**	**a**	**b**		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$p\bar{4}b2$ $(\mathbf{b}'/4)$	L60
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$p\bar{4}b2$ $(\mathbf{b}'/4)$	L60
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d},$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$pba2$ $(\mathbf{b}'/4)$	L25
(110)	**c**	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Fddd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/a$	L07
(011)	**a**	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/b$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L07
	b	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$	$[(\mathbf{a}'+\mathbf{d})/4]$	$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[(\mathbf{a}'+3\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[(3\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L03
$(1\bar{1}0)$	**c**	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$Fddd$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$\widehat{p}112/b$	L07
$(01\bar{1})$	**a**	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$	(origin 2)	$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$\widehat{p}112/a$ $(\mathbf{a}'/4$ or $\mathbf{b}'/4)$	L07
$(\bar{1}01)$	**b**	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$		$[\frac{1}{8}\mathbf{d}, \frac{5}{8}\mathbf{d};$	$c222$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$\frac{3}{8}\mathbf{d}, \frac{7}{8}\mathbf{d}]$	$c222$ $[3(\mathbf{a}'+\mathbf{b}')/8]$	L22
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{4})\mathbf{d};$		
					$(\pm s+\frac{1}{2})\mathbf{d}, (\pm s+\frac{3}{4})\mathbf{d}]$	$\widehat{p}112$ $[(\mathbf{a}'+\mathbf{b}')/8]$	L03
(111)	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\tau/2$	$R\bar{3}c$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d};$	$p\bar{3}$	L66
$(\bar{1}\bar{1}1)$	$-\mathbf{a}-\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\tau_3/2$		$\frac{1}{3}\mathbf{d}, \frac{5}{6}\mathbf{d};$	$p\bar{3}$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L66
$(1\bar{1}\bar{1})$	$\mathbf{a}+\mathbf{c}$	$-\mathbf{a}-\mathbf{b}$	$\tau_1/2$		$\frac{2}{3}\mathbf{d}, \frac{1}{6}\mathbf{d}]$	$p\bar{3}$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L66
$(\bar{1}1\bar{1})$	$\mathbf{c}-\mathbf{a}$	$\mathbf{a}+\mathbf{b}$	$\tau_2/2$		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d};$	$p321$	L68
					$\frac{1}{12}\mathbf{d}, \frac{7}{12}\mathbf{d};$	$p321$ $[(2\mathbf{a}'+\mathbf{b}')/3]$	L68
					$\frac{5}{12}\mathbf{d}, \frac{11}{12}\mathbf{d}]$	$p321$ $[(\mathbf{a}'+2\mathbf{b}')/3]$	L68
					$[\pm s\mathbf{d}, (\pm s+\frac{1}{6})\mathbf{d},$		
					$(\pm s+\frac{1}{3})\mathbf{d}, (\pm s+\frac{1}{2})\mathbf{d},$		
					$(\pm s+\frac{2}{3})\mathbf{d}, (\pm s+\frac{5}{6})\mathbf{d}]$	$p3$	L65

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Auxiliary tables for Laue class $O_h - m\overline{3}m$

Centring type *P*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(nm0)$	$\mathbf{c}$	$m\mathbf{a}-n\mathbf{b}$	$q\mathbf{a}+p\mathbf{b}$			
$(\overline{n}m0)$	$\mathbf{c}$	$m\mathbf{a}+n\mathbf{b}$	$-q\mathbf{a}+p\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\overline{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(0nm)$	$\mathbf{a}$	$m\mathbf{b}-n\mathbf{c}$	$q\mathbf{b}+p\mathbf{c}$			
$(0\overline{n}m)$	$\mathbf{a}$	$m\mathbf{b}+n\mathbf{c}$	$-q\mathbf{b}+p\mathbf{c}$			
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(n0\overline{m})$	$\mathbf{b}$	$n\mathbf{c}+m\mathbf{a}$	$-p\mathbf{c}+q\mathbf{a}$			
$(m0n)$	$\mathbf{b}$	$m\mathbf{c}-n\mathbf{a}$	$q\mathbf{c}+p\mathbf{a}$			
$(m0\overline{n})$	$\mathbf{b}$	$m\mathbf{c}+n\mathbf{a}$	$-q\mathbf{c}+p\mathbf{a}$			
(hhl)	$\mathbf{a}-\mathbf{b}$	$n(\mathbf{a}+\mathbf{b})-m\mathbf{c}$	$p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$
$(\overline{h}\overline{h}l)$	$\mathbf{a}-\mathbf{b}$	$n(\mathbf{a}+\mathbf{b})+m\mathbf{c}$	$-p(\mathbf{a}+\mathbf{b})+q\mathbf{c}$			
$(h\overline{h}l)$	$\mathbf{a}+\mathbf{b}$	$n(\mathbf{b}-\mathbf{a})-m\mathbf{c}$	$p(\mathbf{b}-\mathbf{a})+q\mathbf{c}$	$\mathbf{b}-\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$
$(\overline{h}hl)$	$\mathbf{a}+\mathbf{b}$	$n(\mathbf{b}-\mathbf{a})+m\mathbf{c}$	$-p(\mathbf{b}-\mathbf{a})+q\mathbf{c}$			
(lhh)	$\mathbf{b}-\mathbf{c}$	$n(\mathbf{b}+\mathbf{c})-m\mathbf{a}$	$p(\mathbf{b}+\mathbf{c})+q\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$
$(l\overline{h}\overline{h})$	$\mathbf{b}-\mathbf{c}$	$n(\mathbf{b}+\mathbf{c})+m\mathbf{a}$	$-p(\mathbf{b}+\mathbf{c})+q\mathbf{a}$			
$(lh\overline{h})$	$\mathbf{b}+\mathbf{c}$	$n(\mathbf{c}-\mathbf{b})-m\mathbf{a}$	$p(\mathbf{c}-\mathbf{b})+q\mathbf{a}$	$\mathbf{c}-\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$
$(l\overline{h}h)$	$\mathbf{b}+\mathbf{c}$	$n(\mathbf{c}-\mathbf{b})+m\mathbf{a}$	$-p(\mathbf{c}-\mathbf{b})+q\mathbf{a}$			
(hlh)	$\mathbf{c}-\mathbf{a}$	$n(\mathbf{c}+\mathbf{a})-m\mathbf{b}$	$p(\mathbf{c}+\mathbf{a})+q\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$
$(\overline{h}l\overline{h})$	$\mathbf{c}-\mathbf{a}$	$n(\mathbf{c}+\mathbf{a})+m\mathbf{b}$	$-p(\mathbf{c}+\mathbf{a})+q\mathbf{b}$			
$(\overline{h}lh)$	$\mathbf{c}+\mathbf{a}$	$n(\mathbf{a}-\mathbf{c})-m\mathbf{b}$	$p(\mathbf{a}-\mathbf{c})+q\mathbf{b}$	$\mathbf{a}-\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$
$(hl\overline{h})$	$\mathbf{c}+\mathbf{a}$	$n(\mathbf{a}-\mathbf{c})+m\mathbf{b}$	$-p(\mathbf{a}-\mathbf{c})+q\mathbf{b}$			
l odd $\Rightarrow n=l$, $m=2h$; l even $\Rightarrow n=l/2$, $m=h$						

Arithmetic classes $432P$ and $\bar{4}3mP$

Serial No.	207	208	212	213	215	218
Group type	O^1	O^2	O^6	O^7	T_d^1	T_d^4
Group	$P432$	$P4_232$	$P4_332$	$P4_132$	$P\bar{4}3m$	$P\bar{4}3n$
$(mn0)$	$P112$	$P112$	$P112_1$	$P112_1$	$P112$	$P112$
$(\bar{m}n0)$			$(\mathbf{a}/4)$	$(\mathbf{a}/4)$		
$(nm0)$						
$(\bar{n}m0)$						
$(0mn)$			$P112_1$	$P112_1$		
$(0\bar{m}n)$			$(\mathbf{b}/4)$	$(\mathbf{b}/4)$		
$(0nm)$						
$(0\bar{n}m)$						
$(n0m)$			$P112_1$	$P112_1$		
$(n0\bar{m})$			$(\mathbf{c}/4)$	$(\mathbf{c}/4)$		
$(m0n)$						
$(m0\bar{n})$						
(hhl)	$A112$	$A112$	$A112$	$A112$	$A11m$	$A11a$
$(\bar{h}\bar{h}l)$		$(\mathbf{a}+\mathbf{c})/4$	$(\mathbf{a}+\mathbf{c})/8$	$3(\mathbf{a}+\mathbf{c})/8$		
$(h\bar{h}l)$			$A112$	$A112$		
$(\bar{h}hl)$			$3(\mathbf{b}+\mathbf{c})/8$	$(\mathbf{b}+\mathbf{c})/8$		
(lhh)		$A112$	$A112$	$A112$		
$(l\bar{h}\bar{h})$		$(\mathbf{b}+\mathbf{a})/4$	$(\mathbf{b}+\mathbf{a})/8$	$3(\mathbf{b}+\mathbf{a})/8$		
$(lh\bar{h})$			$A112$	$A112$		
$(l\bar{h}h)$			$3(\mathbf{c}+\mathbf{a})/8$	$(\mathbf{c}+\mathbf{a})/8$		
(hlh)		$A112$	$A112$	$A112$		
$(\bar{h}l\bar{h})$		$(\mathbf{c}+\mathbf{b})/4$	$(\mathbf{c}+\mathbf{b})/8$	$3(\mathbf{c}+\mathbf{b})/8$		
$(\bar{h}lh)$			$A112$	$A112$		
$(hl\bar{h})$			$3(\mathbf{a}+\mathbf{b})/8$	$(\mathbf{a}+\mathbf{b})/8$		

Arithmetic class $m\bar{3}mP$

Serial No. Group type Group	221 O_h^1 $Pm\bar{3}m$	222 O_h^2 $Pn\bar{3}m$		223 O_h^3 $Pm\bar{3}n$	224 O_h^4 $Pn\bar{3}n$	
		Origin 1	Origin 2		Origin 1	Origin 2
$(mn0)$ $(\bar{m}n0)$ $(nm0)$ $(\bar{n}m0)$ $(0mn)$ $(0\bar{m}n)$ $(0nm)$ $(0\bar{n}m)$ $(n0m)$ $(n0\bar{m})$ $(m0n)$ $(m0\bar{n})$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$	$P112/m$	$P112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$P112/n$
(hhl) $(\bar{h}\bar{h}l)$	$A112/m$	$A112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/n$	$A112/n$	$A112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/m$
$(h\bar{h}l)$ $(\bar{h}hl)$		$A112/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/a$		$A112/m$ $(3\mathbf{a}+\mathbf{b}+\mathbf{c})/4$ or $(\mathbf{a}+3\mathbf{b}+\mathbf{c})/4$	$A112/m$ ($\mathbf{a}/2$ or $\mathbf{b}/2$)
(lhh) $(l\bar{h}\bar{h})$		$A112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/n$		$A112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/m$
$(lh\bar{h})$ $(l\bar{h}h)$		$A112/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/a$		$A112/m$ $(\mathbf{a}+3\mathbf{b}+\mathbf{c})/4$ or $(\mathbf{a}+\mathbf{b}+3\mathbf{c})/4$	$A112/m$ ($\mathbf{b}/2$ or $\mathbf{c}/2$)
(hlh) $(\bar{h}l\bar{h})$		$A112/n$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/n$		$A112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/m$
$(\bar{h}lh)$ $(hl\bar{h})$		$A112/a$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/a$		$A112/m$ $(\mathbf{a}+\mathbf{b}+3\mathbf{c})/4$ or $(3\mathbf{a}+\mathbf{b}+\mathbf{c})/4$	$A112/m$ ($\mathbf{c}/2$ or $\mathbf{a}/2$)

Centring type *I*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(mn0)$	$\mathbf{c}$	$n\mathbf{a}-m\mathbf{b}$	$p\mathbf{a}+q\mathbf{b}$	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$
$(\overline{m}n0)$	$\mathbf{c}$	$n\mathbf{a}+m\mathbf{b}$	$-p\mathbf{a}+q\mathbf{b}$			
$(nm0)$	$\mathbf{c}$	$m\mathbf{a}-n\mathbf{b}$	$q\mathbf{a}+p\mathbf{b}$			
$(\overline{n}m0)$	$\mathbf{c}$	$m\mathbf{a}+n\mathbf{b}$	$-q\mathbf{a}+p\mathbf{b}$			
$(0mn)$	$\mathbf{a}$	$n\mathbf{b}-m\mathbf{c}$	$p\mathbf{b}+q\mathbf{c}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$
$(0\overline{m}n)$	$\mathbf{a}$	$n\mathbf{b}+m\mathbf{c}$	$-p\mathbf{b}+q\mathbf{c}$			
$(0nm)$	$\mathbf{a}$	$m\mathbf{b}-n\mathbf{c}$	$q\mathbf{b}+p\mathbf{c}$			
$(0\overline{n}m)$	$\mathbf{a}$	$m\mathbf{b}+n\mathbf{c}$	$-q\mathbf{b}+p\mathbf{c}$			
$(n0m)$	$\mathbf{b}$	$n\mathbf{c}-m\mathbf{a}$	$p\mathbf{c}+q\mathbf{a}$	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$
$(n0\overline{m})$	$\mathbf{b}$	$n\mathbf{c}+m\mathbf{a}$	$-p\mathbf{c}+q\mathbf{a}$			
$(m0n)$	$\mathbf{b}$	$m\mathbf{c}-n\mathbf{a}$	$q\mathbf{c}+p\mathbf{a}$			
$(m0\overline{n})$	$\mathbf{b}$	$m\mathbf{c}+n\mathbf{a}$	$-q\mathbf{c}+p\mathbf{a}$			
(hhl)	$\mathbf{a}-\mathbf{b}$	$n\widehat{\mathbf{a}}-m\mathbf{c}$	$p\widehat{\mathbf{a}}+q\mathbf{c}$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$
$(\overline{h}hl)$	$\mathbf{a}-\mathbf{b}$	$n\widehat{\mathbf{a}}+m\mathbf{c}$	$-p\widehat{\mathbf{a}}+q\mathbf{c}$			
$(h\overline{h}l)$	$\mathbf{a}+\mathbf{b}$	$n\widehat{\mathbf{a}}-m\mathbf{c}$	$p\widehat{\mathbf{a}}+q\mathbf{c}$	$(\mathbf{b}-\mathbf{a}+\mathbf{c})/2$	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$
$(\overline{h}hl)$	$\mathbf{a}+\mathbf{b}$	$n\widehat{\mathbf{a}}+m\mathbf{c}$	$-p\widehat{\mathbf{a}}+q\mathbf{c}$			
(lhh)	$\mathbf{b}-\mathbf{c}$	$n\widehat{\mathbf{a}}-m\mathbf{a}$	$p\widehat{\mathbf{a}}+q\mathbf{a}$	$(\mathbf{b}+\mathbf{c}+\mathbf{a})/2$	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$
$(l\overline{h}h)$	$\mathbf{b}-\mathbf{c}$	$n\widehat{\mathbf{a}}+m\mathbf{a}$	$-p\widehat{\mathbf{a}}+q\mathbf{a}$			
$(lh\overline{h})$	$\mathbf{b}+\mathbf{c}$	$n\widehat{\mathbf{a}}-m\mathbf{a}$	$p\widehat{\mathbf{a}}+q\mathbf{a}$	$(\mathbf{c}-\mathbf{b}+\mathbf{a})/2$	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$
$(l\overline{h}h)$	$\mathbf{b}+\mathbf{c}$	$n\widehat{\mathbf{a}}+m\mathbf{a}$	$-p\widehat{\mathbf{a}}+q\mathbf{a}$			
(hlh)	$\mathbf{c}-\mathbf{a}$	$n\widehat{\mathbf{a}}-m\mathbf{b}$	$p\widehat{\mathbf{a}}+q\mathbf{b}$	$(\mathbf{c}+\mathbf{a}+\mathbf{b})/2$	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$
$(\overline{h}l\overline{h})$	$\mathbf{c}-\mathbf{a}$	$n\widehat{\mathbf{a}}+m\mathbf{b}$	$-p\widehat{\mathbf{a}}+q\mathbf{b}$			
$(\overline{h}lh)$	$\mathbf{c}+\mathbf{a}$	$n\widehat{\mathbf{a}}-m\mathbf{b}$	$p\widehat{\mathbf{a}}+q\mathbf{b}$	$(\mathbf{a}-\mathbf{c}+\mathbf{b})/2$	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$
$(hl\overline{h})$	$\mathbf{c}+\mathbf{a}$	$n\widehat{\mathbf{a}}+m\mathbf{b}$	$-p\widehat{\mathbf{a}}+q\mathbf{b}$			
l odd $\Rightarrow n=2l, m=2h+l$; l even $\Rightarrow n=l, m=h+l/2$						

Arithmetic classes $432I$, $\overline{4}3mI$ and $m\overline{3}mI$

Serial No.	211	214	217	220	229	230
Group type	O^5	O^8	T_d^3	T_d^6	O_h^9	O_h^{10}
Group	$I432$	$I4_132$	$I\overline{4}3m$	$I\overline{4}3d$	$Im\overline{3}m$	$Ia\overline{3}d$
$(mn0)$	$I112$	$I112$	$I112$	$I112$	$I112/m$	$I112/b$
$(\overline{m}n0)$		$(\mathbf{b}/4)$		$(\mathbf{b}/4)$		
$(nm0)$						
$(\overline{n}m0)$						
$(0mn)$		$I112$		$I112$		
$(0\overline{m}n)$		$(\mathbf{c}/4)$		$(\mathbf{c}/4)$		
$(0nm)$						
$(0\overline{n}m)$						
$(n0m)$		$I112$		$I112$		
$(n0\overline{m})$		$(\mathbf{a}/4)$		$(\mathbf{a}/4)$		
$(m0n)$						
$(m0\overline{n})$						
(hhl)	$B112$	$B112$	$B11m$	$B11b$	$B112/m$	$B112/b$
$(\overline{h}\overline{h}l)$		$(\mathbf{a}+\mathbf{c})/8$				
$(h\overline{h}l)$		$B112$				
$(\overline{h}hl)$		$3(\mathbf{a}+\mathbf{c})/8$				
(lhh)		$B112$				
$(l\overline{h}\overline{h})$		$(\mathbf{b}+\mathbf{a})/8$				
$(lh\overline{h})$		$B112$				
$(l\overline{h}h)$		$3(\mathbf{b}+\mathbf{a})/8$				
(hlh)		$B112$				
$(\overline{h}l\overline{h})$		$(\mathbf{c}+\mathbf{b})/8$				
$(\overline{h}lh)$		$B112$				
$(hl\overline{h})$		$3(\mathbf{c}+\mathbf{b})/8$				

Centring type *F*

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Auxiliary basis of the scanning group $\widehat{\mathbf{a}}$	$\widehat{\mathbf{b}}$	$\widehat{\mathbf{c}}$
$(hk0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$
$(\overline{h}k0)$	$\mathbf{c}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
$(kh0)$	$\mathbf{c}$	$m\widehat{\mathbf{a}} + n\mathbf{b}$	$q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
$(\overline{k}h0)$	$\mathbf{c}$	$m\widehat{\mathbf{a}} - n\widehat{\mathbf{b}}$	$-q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
$(0hk)$	$\mathbf{a}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$
$(0\overline{h}k)$	$\mathbf{a}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
$(0kh)$	$\mathbf{a}$	$m\widehat{\mathbf{a}} - n\widehat{\mathbf{b}}$	$q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
$(0\overline{k}h)$	$\mathbf{a}$	$m\widehat{\mathbf{a}} + n\widehat{\mathbf{b}}$	$-q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
$(k0h)$	$\mathbf{b}$	$n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$	$p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$
$(k0\overline{h})$	$\mathbf{b}$	$n\widehat{\mathbf{a}} + m\widehat{\mathbf{b}}$	$-p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$			
$(h0k)$	$\mathbf{b}$	$m\widehat{\mathbf{a}} - n\widehat{\mathbf{b}}$	$q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
$(h0\overline{k})$	$\mathbf{b}$	$m\widehat{\mathbf{a}} + n\widehat{\mathbf{b}}$	$-q\widehat{\mathbf{a}} + p\widehat{\mathbf{b}}$			
h even, k odd or h odd, k even $\Rightarrow n = h+k$, $m = h-k$ h, k odd $\Rightarrow n = (h+k)/2$, $m = (h-k)/2$						
(hhl)	$(\mathbf{a}-\mathbf{b})/2$	$n\widehat{\mathbf{a}} - m\mathbf{c}$	$p\widehat{\mathbf{a}} + q\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$
$(\overline{h}\overline{h}l)$	$(\mathbf{a}-\mathbf{b})/2$	$n\widehat{\mathbf{a}} + m\mathbf{c}$	$-p\widehat{\mathbf{a}} + q\mathbf{c}$			
$(h\overline{h}l)$	$(\mathbf{a}+\mathbf{b})/2$	$n\widehat{\mathbf{a}} - m\mathbf{c}$	$p\widehat{\mathbf{a}} + q\mathbf{c}$	$(\mathbf{b}-\mathbf{a})/2$	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$
$(\overline{h}hl)$	$(\mathbf{a}+\mathbf{b})/2$	$n\widehat{\mathbf{a}} + m\mathbf{c}$	$-p\widehat{\mathbf{a}} + q\mathbf{c}$			
(lhh)	$(\mathbf{b}-\mathbf{c})/2$	$n\widehat{\mathbf{a}} - m\mathbf{a}$	$p\widehat{\mathbf{a}} + q\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$
$(l\overline{h}\overline{h})$	$(\mathbf{b}-\mathbf{c})/2$	$n\widehat{\mathbf{a}} + m\mathbf{a}$	$-p\widehat{\mathbf{a}} + q\mathbf{a}$			
$(lh\overline{h})$	$(\mathbf{b}+\mathbf{c})/2$	$n\widehat{\mathbf{a}} - m\mathbf{a}$	$p\widehat{\mathbf{a}} + q\mathbf{a}$	$(\mathbf{c}-\mathbf{b})/2$	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$
$(l\overline{h}h)$	$(\mathbf{b}+\mathbf{c})/2$	$n\widehat{\mathbf{a}} + m\mathbf{a}$	$-p\widehat{\mathbf{a}} + q\mathbf{a}$			
(hlh)	$(\mathbf{c}-\mathbf{a})/2$	$n\widehat{\mathbf{a}} - m\mathbf{b}$	$p\widehat{\mathbf{a}} + q\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$
$(\overline{h}l\overline{h})$	$(\mathbf{c}-\mathbf{a})/2$	$n\widehat{\mathbf{a}} + m\mathbf{b}$	$-p\widehat{\mathbf{a}} + q\mathbf{b}$			
$(\overline{h}lh)$	$(\mathbf{c}+\mathbf{a})/2$	$n\widehat{\mathbf{a}} - m\mathbf{b}$	$p\widehat{\mathbf{a}} + q\mathbf{b}$	$(\mathbf{a}-\mathbf{c})/2$	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$
$(hl\overline{h})$	$(\mathbf{c}+\mathbf{a})/2$	$n\widehat{\mathbf{a}} + m\mathbf{b}$	$-p\widehat{\mathbf{a}} + q\mathbf{b}$			
h odd $\Rightarrow m = h$, $n = 2l$; h even $\Rightarrow m = h/2$, $n = l$						

Arithmetic classes $432F$ and $\bar{4}3mF$

Serial No.	209	210	216	219
Group type	O^3	O^4	T_d^2	T_d^5
Group	$F432$	$F4_132$	$F\bar{4}3m$	$F\bar{4}3c$
$(hk0)$ $(\bar{h}k0)$ $(kh0)$ $(\bar{k}h0)$ $(0hk)$ $(0\bar{h}k)$ $(0kh)$ $(0\bar{k}h)$ $(k0h)$ $(k0\bar{h})$ $(h0k)$ $(h0\bar{k})$	$I112$	$I112$	$I112$	$I112$
(hhl) $(\bar{h}\bar{h}l)$	$I112$	$I112$ $(\mathbf{a}/4+\mathbf{c}/8)$	$I11m$	$I11a$
$(h\bar{h}l)$ $(\bar{h}hl)$		$I112$ $(\mathbf{a}/4+3\mathbf{c}/8)$		$I11b$
(lhh) $(l\bar{h}\bar{h})$		$I112$ $(\mathbf{b}/4+\mathbf{a}/8)$		$I11a$
$(lh\bar{h})$ $(l\bar{h}h)$		$I112$ $(\mathbf{b}/4+3\mathbf{a}/8)$		$I11b$
(hlh) $(\bar{h}l\bar{h})$		$I112$ $(\mathbf{c}/4+\mathbf{b}/8)$		$I11a$
$(\bar{h}lh)$ $(hl\bar{h})$		$I112$ $(\mathbf{c}/4+3\mathbf{b}/8)$		$I11b$

Arithmetic class $m\overline{3}mF$

Serial No.	225	226	227		228	
Group type	O_h^5	O_h^6	O_h^7		O_h^8	
Group	$Fm\overline{3}m$	$Fm\overline{3}c$	$Fd\overline{3}m$		$Fd\overline{3}c$	
			Origin 1	Origin 2	Origin 1	Origin 2
$(hk0)$ $(\overline{h}k0)$ $(kh0)$ $(\overline{k}h0)$ $(0hk)$ $(0\overline{h}k)$ $(0kh)$ $(0\overline{k}h)$ $(k0h)$ $(k0\overline{h})$ $(h0k)$ $(h0\overline{k})$	$I112/m$	$I112/m$	$I112/b$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/b$	$I112/b$ $3(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/b$
(hhl) $(\overline{h}\overline{h}l)$	$I112/m$	$I112/a$	$I112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/m$	$I112/a$ $3(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/a$
$(h\overline{h}l)$ $(\overline{h}hl)$			$I112/m$ $(\mathbf{a}+3\mathbf{b}+3\mathbf{c})/8$ or $(3\mathbf{a}+\mathbf{b}+3\mathbf{c})/8$	$I112/m$ $(\mathbf{a}+\mathbf{c})/4$ or $(\mathbf{b}+\mathbf{c})/4$	$I112/a$ $(\mathbf{a}+3\mathbf{b}+\mathbf{c})/8$ or $(3\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/a$ $(\mathbf{a}+\mathbf{c})/4$ or $(\mathbf{b}+\mathbf{c})/4$
(lhh) $(l\overline{h}\overline{h})$			$I112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/m$	$I112/a$ $3(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/a$
$(lh\overline{h})$ $(l\overline{h}h)$			$I112/m$ $(3\mathbf{a}+\mathbf{b}+3\mathbf{c})/8$ or $(3\mathbf{a}+3\mathbf{b}+\mathbf{c})/8$	$I112/m$ $(\mathbf{b}+\mathbf{a})/4$ or $(\mathbf{c}+\mathbf{a})/4$	$I112/a$ $(\mathbf{a}+\mathbf{b}+3\mathbf{c})/8$ or $(\mathbf{a}+3\mathbf{b}+\mathbf{c})/8$	$I112/a$ $(\mathbf{b}+\mathbf{a})/4$ or $(\mathbf{c}+\mathbf{a})/4$
(hlh) $(\overline{h}l\overline{h})$			$I112/m$ $(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/m$	$I112/a$ $3(\mathbf{a}+\mathbf{b}+\mathbf{c})/8$	$I112/a$
$(\overline{h}lh)$ $(hl\overline{h})$			$I112/m$ $(3\mathbf{a}+3\mathbf{b}+\mathbf{c})/8$ or $(\mathbf{a}+3\mathbf{b}+3\mathbf{c})/8$	$I112/m$ $(\mathbf{c}+\mathbf{b})/4$ or $(\mathbf{a}+\mathbf{b})/4$	$I112/a$ $(3\mathbf{a}+\mathbf{b}+\mathbf{c})/8$ or $(\mathbf{a}+\mathbf{b}+3\mathbf{c})/8$	$I112/a$ $(\mathbf{c}+\mathbf{b})/4$ or $(\mathbf{a}+\mathbf{b})/4$

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